TA-nummer
2944/2012

PFOA Isomers, Salts and Precursors

Literature study and evaluation of physico-chemical properties.

Klif project no. 3012013

Claus Jørgen Nielsen
CTCC, Department of Chemistry
University of Oslo

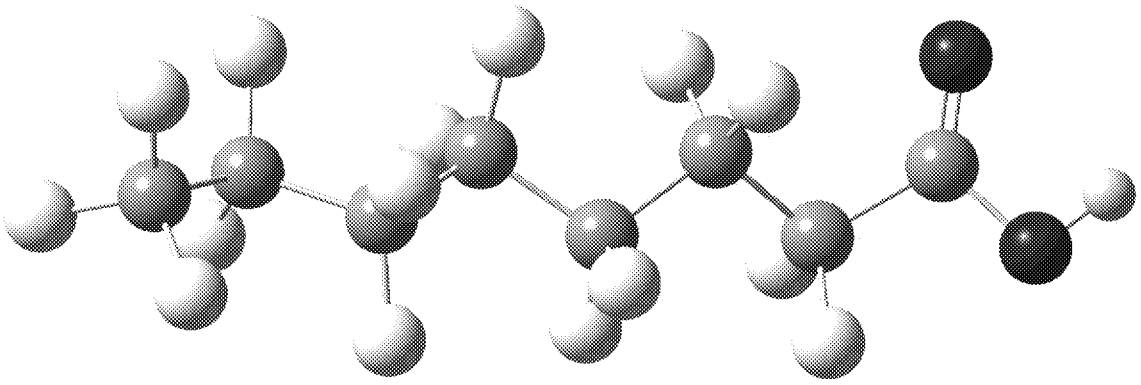
This page is intentionally left blank

PFOA Isomers, Salts and Precursors

Literature study and evaluation of physico-chemical properties.

Claus Jørgen Nielsen

CTCC, Department of Chemistry, University of Oslo



Structure of gaseous PFOA as resulting from quantum chemistry calculations.

Preface

Klif, in cooperation with German Environment Authorities, is preparing a report proposing regulations on PFOA (perfluorooctanoic acid), its salts and precursors. PFOA (or its ammonium salt), is mainly used as a processing aid in the production of fluoropolymers; i.e. polytetrafluoroethylene (PTFE) and polyvinylidenefluoride (PVDF). Other PFOA sources are fluorotelomers, which are not produced using PFOA, but which may contain low levels of PFOA. There are a number of products containing PFOA such as carpet care solutions, sealants, floor waxes, paints, impregnating agents, fire fighting foam, ski wax and surface coatings of carpets, textiles, paper and leather. PFOA is found in the environment and in people all over the world. PFOA is degraded very slowly in nature and is long-range transported to the Arctic. PFOA is listed as a priority pollutant covered by the national goal that emissions should be eliminated by 2020.

The overall objective of the present project is to summarize relevant information available in the open literature and to sketch how missing and necessary data for an environmental impact assessment can be provided. The specific objectives are:

1. To summarize physico-chemical data for
    a. Branched perfluorooctanoic acid (PFOA); CAS no 90480-55-0
    b. Ammonium salt of branced PFOA (APFO); CAS no 90480-56-1
    c. Sodium salt of PFOA; CAS No. 335-95-5
    d. Potassium salt of PFOA; CAS No. 2395-00-8
    e. Silver salt of PFOA; CAS No. 335-93-3

2. To evaluate routes for obtaining missing critical data, including expert evaluations of these data

3. To provide an overall assessment of relevant precursors including possible lumping into groups, and to evaluate possible routes to provide documentation, where missing, on the potential of abiotic degradation resulting in PFOA

The present report summarises the physico-chemical data for PFOA isomers and salts available in the open literature, and a classification of PFOA precursors.

The project has achieved its targets.

This page is intentionally left blank

Table of Contents

Executive Summary

The literature on PFOA including its structural isomers and their ammonium, sodium, potassium and silver salts referenced in CAS[#] registry database has been reviewed with respect to physico-chemical properties.
There are 11 structural isomers of PFOA registered in CAS. Of these there are experimental physico-chemical data available for unbranched PFOA ($CF_3(CF_2)_6COOH$) and for $(CF_3)_2CF(CF_2)_4COOH$. Witin experimental and model uncertainties all PFOA isomers have comparable physico-chemical properties: the vapour pressures are around 4 Pa at 25 °C, the melting points are in the range 13-55 °C, the boiling points are around 190 °C at 1 atm, and the water solubilities are more than 1 g/L at the critical micelle concentration.

It is difficult to determine pK_a for PFOA experimentally, however available data supports that the acid strength of PFOA and branched PFOA isomers will be somewhere between pK_a = 1.8 and 2.8.. Assuming a pK_a of 2.8, more than 99% of aqueous PFOA exists as its anionic form at typical environmental pH of 5–8. Experiments, carried out in aqueous ethanol and methanol solutions suggest a pK_a value of 2.8 and 3.5, while results from titrations of CF_3COOH, CF_3CF_2COOH and $CF_3CF_2CF_2COOH$ in aqueous solutions and quantum chemistry based calculations suggest a lower value. Partitioning of PFOA in the environment strongly depends on its acid strength. If it turns out that higher accuracy of PFOA partitioning is needed in environmental impact assessment studies, a systematic theoretical study of PFCA and PFOA acid strengths could be undertaken. This would imply a systematic theoretical study of the acid strengths of PFOA, CF_3COOH, CF_3CF_2COOH and $CF_3CF_2CF_2COOH$ employing data for the latter three PFCAs as anchor points.

The solubility of the the ammonium, sodium, potassium and silver salts of PFOA are all reasonably soluble in water – the silver salt is the least soluble, $K_{sp} \approx 10^{-5}$ M^2 (>1 g/L). The PFOA salts are stable at environmental conditions. However, they all decompose at elevated temperatures. The thermal stability and decomposition of the salts differ; the ammonium salt will likely decompose to give $NH_3 + CO_2 + CF_3(CF_2)_6CF_2H$ (thermal decomposition of $C_3F_7CO_2NH_4$ gives $CF_3CF_2CF_2H + CO_2 + NH_3$). The sodium salt decomposes to give $CF_3(CF_2)_nCF=CF_2 + CO_2 + NaF$, while the silver salt decomposes to give $C_{14}F_{30}$. There are no data reported for the thermal degradation products of the potassium salt, but it will likely decompose in a similar way as the sodium salt and give $CF_3(CF_2)_nCF=CF_2 + CO_2 + KF$.

[#] CAS, Chemical Abstract Service

This page is intentionally left blank

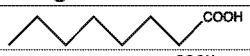
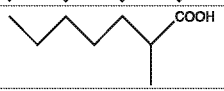
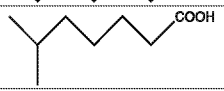
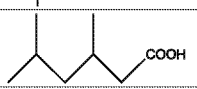
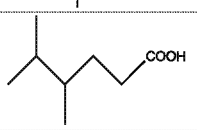
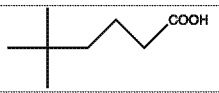
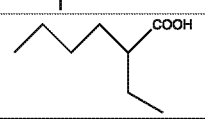
1 Literature study of PFOA, PFOA isomers and selected PFOA salts

The literature on PFOA including its structural isomers and their ammonium, sodium, potassium and silver salts referenced in CAS by 11.03.2012 and other publicly available information, including data on www, has been examined.

1.1 Physico-chemical data for PFOA and PFOA isomers

The CAS Registry Number 90480-55-0 is a generic registration number that covers all branched pentadecafluoro octanoic acids (the number itself cannot be used for search in the CAS database). There are 39 possible structural isomers of pentadecafluoro octanoic acid (1 with chain length 8, 5 with chain length 7, 13 with chain length 6, 16 with chain length 5, and 4 with chain length 4). Only 10 of these are registered in CAS with references, **Table 1.1**. Branched pentadeca octanoic acid is listed as no. 291-790-8 in the European Inventory of Existing Commercial chemical Substances (EINECS).

Table 1.1. Summary of CAS Registry information on compounds with formula $C_8HF_{15}O$.

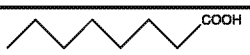
Chain length and Structure	CAS Registry Number	Notes.
8 	335-67-1	More than 2200 references listed.
7 	207678-51-1	5 references listed in CAS.
7 	705240-04-6	6 references listed in CAS.
7 	1144512-18-4	6 references listed in CAS.
7 	909009-42-3	7 references listed in CAS.
7 	15166-06-0	16 references listed in CAS.
6 	1144512-35-5	2 references listed in CAS.
6 	1192593-79-5	1 reference listed in CAS.
6 	1144512-36-6	2 references listed in CAS.
6 	1144512-34-4	2 references listed in CAS.
6 	35605-76-6	6 references listed in CAS.

1.1.1 CAS Registry Number 335-67-1

There are more than 100 commercial sources of PFOA[#] (CAS RN 335-67-1, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Pentadecafluoro-octanoic acid) and more than 2200 references are listed in CAS. Nearly 500 of these are linked to patents and nearly 700 are concerned with biological studies.

Less than 200 of the references listed in CAS deals with various molecular properties. **Table 1.2** compares experimental and calculated physico-chemical data for PFOA. The comparison provides a basis for an evaluation of model results for the branched PFOAs; see section 1.1.12, page 19). The linear PFOA isomer is often abbreviated n-PFOA to distinguish it from its branched isomers.

Table 1.2. Overview of physico-chemical properties for PFOA isomer 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-octanoic acid, CAS Number 335-67-1.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	Solid	[*Kauck and Diesslin*, 1951]
Melting/freezing point	54.9-55.6 °C 40 °C sublimation	[*Hare et al.*, 1954] [*Bernett and Zisman*, 1959] [*Nakayama*, 1967]
Boiling point	189°C at 98.1 kPa 188°C at 101.3 kPa	[*Kauck and Diesslin*, 1951] Calculated [a]
Vapour pressure at 25 °C	4.0 Pa 4.2 Pa 4.1 Pa 37 Pa	[*Kaiser et al.*, 2005] [*Washburn et al.*, 2005] [*Barton et al.*, 2008] Calculated [a]
Water solubility at c.m.c. [b] Water solubility, saturated solution	0.0090 mol/L at 20 °C 0.023 mol/L at 25 °C 13 g/L, 0.032 mol/L 4.14 g/L at 22°C	[*Shinoda et al.*, 1972] [*Kauck and Diesslin*, 1951] Calculated [a] [*Prokop et al.*, 1989][g]
Partition coefficient n-octanol/water (log value)	2.69 at pH=7 and 25°C 6.3	Calculated [a] EPI [h]
Dissociation constant	pKa = 2.8 ± 0.03 [c] pKa = 2.14 ± 0.06 [d] pKa = 3.8 ± 0.1 [e] pKa = -0.5 [f] pKa =-0.47 ± 0.10	[*Brace*, 1962] [*Radell et al.*, 1965] [*Burns et al.*, 2008] Estimated, [*Goss*, 2008] Calculated [a]
Henry's Law constant (mol dm^{-3} atm^{-1})	9.9 ±1.5 for pKa =2.8 5.0 ± 0.2 for pKa = 1.3	[*Kutsuna and Hori*, 2008]
Gas/Particle partitioning coefficient (log value)	-2.75 , -1.92	Calculated [*Arp and Goss*, 2009]

[a] From CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] c.m.c., Critical micelle concentration. [c] From titration of PFOA in 50% aqueous ethanol. [d] From titration of PFOA in 95% aqueous ethanol [e] From titration of PFOA in 10-30% aqueous methanol. [f] Estimated on the basis of experimental data for CF_3COOH, other fluorinated

[#] SMILES: O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

carboxylic acids and comparison with theoretically calculated acid strengths. [g] Information presented as: "personal communication, Chung-Ho Wu, The China Petrochemical Development Company, Taiwan. [h] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

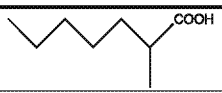
1.1.2 CAS Registry Number 207678-51-1

No commercial sources are listed in CAS for the PFOA isomer 2,3,3,4,4,5,5,6,6,7,7,7-dodecafluoro-2-(trifluoromethyl)-heptanoic acid[#] (CAS Registry Number 207678-51-1). The isomer is also labelled 2m-PFOA.

The references listed in CAS refer to patents [*W-Q Fan and Manzara*, 1998; *Manzara et al.*, 1998; *Stern and Fan*, 1998], a conference contribution describing analysis of LC/ESI-MS/MS spectra of a series of PFOA isomers [*Arsenault et al.*, 2008], and a theoretical study of pKa values of perfluoroalkyl carboxylic acids [*Rayne and Forest*, 2010].

There are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.3** summarises theoretical data listed in CAS.

Table 1.3. Overview of physico-chemical properties for PFOA isomer 2,3,3,4,4,5,5,6,6,7,7,7-dodeca-fluoro-2-(trifluoromethyl)-heptanoic acid, CAS Number 207678-51-1.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa		
Melting/freezing point		
Boiling point at 101.3 kPa	188°C	Calculated [a]
Vapour pressure at 25 °C	37 Pa	Calculated [a]
Water solubility at pH = 7 and 25°C	13 g/L, 0.032 mol/L	Calculated [a]
Partition coefficient n-octanol/water (log value)	2.69 at pH=7 and 25°C 5.59	Calculated [a] EPI [b]
Dissociation constant	pKa =-0.47 ± 0.10	Calculated [a]

[a] From CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

[#] SMILES: O=C(O)C(F)(C(F)(F)(F))C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

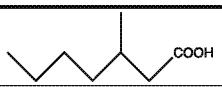
1.1.3 CAS Registry Number 705240-04-6

No commercial sources are listed in CAS for PFOA isomer 2,2,3,4,4,5,5,6,6,7,7,7-dodecafluoro-3-(trifluoromethyl)-heptanoic acid[#] (CAS Registry Number 705240-04-6). The isomer is also labelled 3m-PFOA.

The references listed in CAS refer to toxicology studies [*Benskin et al.*, 2009; *Amilia O. De Silva et al.*, 2009], field measurements [*Amila O. De Silva et al.*, 2009; *Benskin et al.*, 2012], a conference contribution describing analysis of LC/ESI-MS/MS spectra of a series of PFOA isomers [*Arsenault et al.*, 2008], and a theoretical study of pKa values of perfluoroalkyl carboxylic acids [*Rayne and Forest*, 2010].

There are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.4** summarises theoretical data listed in CAS.

Table 1.4. Overview of physico-chemical properties for PFOA isomer 2,2,3,4,4,5,5,6,6,7,7,7-dodeca-fluoro-3-(trifluoromethyl)-heptanoic acid, CAS Number 705240-04-6.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa		
Melting/freezing point		
Boiling point at 760 Torr	170.4 ± 35.0 °C	Calculated [a]
Vapour pressure at 25°C	97 Pa	Calculated [a]
Water solubility at pH = 7 and 25°C	9.5 g/L, 0.023 mol/L	Calculated [a]
Partition coefficient n-octanol/water (log value)	3.09 at pH = 7 and 25°C 5.59	Calculated [a] EPI [b]
Dissociation constant at 25°C	pKa = 0.29 ± 0.10	Calculated [a]

[a] From CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

[#] SMILES: O=C(O)C(F)(F)C(F)(C(F)(F)(F))C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

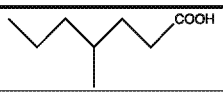
1.1.4 CAS Registry Number 1144512-18-4

No commercial sources are listed in CAS for PFOA isomer 2,2,3,3,4,5,5,6,6,7,7,7-dodecafluoro-4-(trifluoromethyl)-heptanoic acid[#] (CAS Registry Number 1144512-18-4). The isomer is also labelled 4m-PFOA.

The references listed in CAS refer to toxicology studies [*Benskin et al.*, 2009; *Amilia O. De Silva et al.*, 2009], field measurements [*Amila O. De Silva et al.*, 2009; *Benskin et al.*, 2012], a conference contribution describing analysis of LC/ESI-MS/MS spectra of a series of PFOA isomers [*Arsenault et al.*, 2008], to field measurements [*Amila O. De Silva et al.*, 2009; *Benskin et al.*, 2012], and a theoretical study of pKa values of perfluoroalkyl carboxylic acids [*Rayne and Forest*, 2010].

There are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.5** summarises theoretical data listed in CAS.

Table 1.5. Overview of physico-chemical properties for PFOA isomer 2,2,3,3,4,5,5,6,6,7,7,7-dodeca-fluoro-4-(trifluoromethyl)-heptanoic acid, CAS Number 1144512-18-4.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa		
Melting/freezing point		
Boiling point at 760 Torr	172.5 ± 35.0 °C	Calculated [a]
Vapour pressure at 25°C	86 Pa	Calculated [a]
Water solubility at pH = 7 and 25°C	9.5 g/L, 0.023 mol/L	Calculated [a]
Partition coefficient n-octanol/water (log value)	3.07 at pH = 7 and 25°C 5.59	Calculated [a] EPI [b]
Dissociation constant at 25°C	pKa = 0.29 ± 0.10	Calculated [a]

[a] From CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

[#] SMILES: O=C(O)C(F)(F)C(F)(F)C(F)(C(F)(F)(F))C(F)(F)C(F)(F)C(F)(F)F

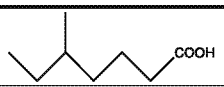
1.1.5 CAS Registry Number 909009-42-3

No commercial sources are listed in CAS for PFOA isomer 2,2,3,3,4,5,5,6,6,7,7,7-dodecafluoro-4-(trifluoromethyl)-heptanoic acid[#] (CAS Registry Number 909009-42-3). The isomer is also labelled 5m-PFOA.

The references listed in CAS refer to toxicology studies [*Vanden et al.*, 2006; *Benskin et al.*, 2009; *Amilia O. De Silva et al.*, 2009], to field measurements [*Amila O. De Silva et al.*, 2009; *Benskin et al.*, 2012], a conference contribution describing analysis of LC/ESI-MS/MS spectra of a series of PFOA isomers [*Arsenault et al.*, 2008], and a theoretical study of pKa values of perfluoroalkyl carboxylic acids [*Rayne and Forest*, 2010].

There are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.6** summarises theoretical data listed in CAS.

Table 1.6. Overview of physico-chemical properties for PFOA isomer 2,2,3,3,4,5,5,6,6,7,7,7–dodeca-fluoro-4-(trifluoromethyl)-heptanoic acid, CAS Number 909009-42-3.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa		
Melting/freezing point		
Boiling point at 760 Torr	173.5 ± 35.0 °C	Calculated [a]
Vapour pressure at 25°C	82 Pa	Calculated [a]
Water solubility at pH = 7 and 25°C	6.6 g/L, 0.016 mol/L	Calculated [a]
Partition coefficient n-octanol/water (log value)	4.35 at pH = 7 and 25°C 5.59	Calculated [a] EPI [b]
Dissociation constant at 25°C	pKa = 0.34 ± 0.10	Calculated [a]

[a] From CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

[#] SMILES: O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)(F))C(F)(F)C(F)(F)F

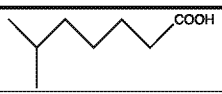
1.1.6 CAS Registry Number 15166-06-0

No commercial sources are listed in CAS for PFOA isomer 2,2,3,3,4,4,5,5,6,7,7,7-dodecafluoro-6-(trifluoromethyl)-heptanoic acid[#] (CAS Registry Number 15166-06-0). The isomer is also labelled 6m-PFOA.

The references listed in CAS refer to patents [*Daikin Kogyo Co Ltd*, 1967; *Katsushima et al.*, 1968; *Hato and Shinoda*, 1970; *Shinoda et al.*, 1972; *Plashkin et al.*, 1975; *Katsushima et al.*, 1976; *Von Werner and Probst*, 1987; *Nishiyama*, 1988; *Yamada and Higaki*, 1993; *Meissner et al.*, 2003; *Wroblewska et al.*, 2006], to toxicology studies [*Benskin et al.*, 2009; *Amilia O. De Silva et al.*, 2009], to field measurements [*Benskin et al.*, 2012], to a conference contribution describing analysis of LC/ESI-MS/MS spectra of a series of PFOA isomers [*Arsenault et al.*, 2008], and a theoretical study of pKa values of perfluoroalkyl carboxylic acids [*Rayne and Forest*, 2010].

Besides 2 boiling point measurements there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.7** summarises experimental and theoretical data listed in CAS.

Table 1.7. Overview of physico-chemical properties for PFOA isomer 2,2,3,3,4,4,5,5,6,7,7,7-dodeca-fluoro-6-(trifluoromethyl)-heptanoic acid, CAS Number 15166-06-0.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa		
Melting/freezing point	13-14 °C	[*Shinoda et al.*, 1972]
Boiling point at 760 Torr	169.4 ± 35.0 °C 189 °C 85-88°C at 6-8 Torr	Calculated [a] [*Wroblewska et al.*, 2006] [*Daikin Kogyo Co Ltd*, 1967]
Vapour pressure at 25°C	102 Pa	Calculated [a]
Water solubility at c.m.c. [b]	0.0085 mol/L at 25°C 6.6 g/L, 0.016 mol/L	[*Shinoda et al.*, 1972] Calculated [a]
Partition coefficient n-octanol/water (log value)	2.85 at pH = 7 and 25°C 5.59	Calculated [a] EPI [c]
Dissociation constant at 25°C	pKa = 0.51 ± 0.10	Calculated [a]

[a] At pH = 7 and 25°C from CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] c.m.c., critical micelle concentration. [c] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

[#] SMILES: O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)(F))C(F)(F)F

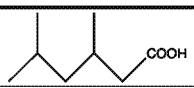
1.1.7 CAS Registry Number 1144512-35-5

No commercial sources are listed in CAS. Physico-chemical data for PFOA isomer 2,2,3,4,4,5,6,6,6-nonafluoro-3,5-bis(trifluoromethyl)-hexanoic acid[#] (CAS Registry Number 1144512-35-5).

The references listed in CAS refer to a toxicology study [*Benskin et al.*, 2009], and to a conference contribution describing analysis of LC/ESI-MS/MS spectra of a series of PFOA isomers [*Arsenault et al.*, 2008].

There are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.8** summarises theoretical data listed in CAS.

Table 1.8. Overview of physico-chemical properties for PFOA isomer 2,2,3,4,4,5,6,6,6-nonafluoro-3,5-bis(trifluoromethyl)-hexanoic acid, CAS Number 1144512-35-5.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa		
Melting/freezing point		
Boiling point at 760 Torr	160.1 ± 35.0°C	Calculated [a]
Vapour pressure at 25°C	168 Pa	Calculated [a]
Water solubility at pH = 7 and 25°C	12 g/L, 0.028 mol/L	Calculated [a]
Partition coefficient n-octanol/water (log value)	2.83 at pH = 7 and 25°C 4.89	Calculated [a] EPI [b]
Dissociation constant at 25°C	pKa = 0.31 ± 0.10	Calculated [a]

[a] From CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

[#] SMILES: O=C(O)C(F)(F)C(F)(C(F)(F)(F))C(F)(F)C(F)(C(F)(F)(F))C(F)(F)F

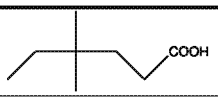
1.1.8 CAS Registry Number 1192593-79-5

No commercial sources are listed in CAS. [*Arsenault et al.*, 2008] Physico-chemical data for PFOA isomer 2,2,3,3,5,5,6,6,6-nonafluoro-4,4-bis(trifluoromethyl)-hexanoic acid[#] (CAS Registry Number 1192593-79-5).

The references listed in CAS refer to a conference contribution describing analysis of LC/ESI-MS/MS spectra of a series of PFOA isomers [*Arsenault et al.*, 2008].

There are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.9** summarises theoretical data listed in CAS.

Table 1.9. Overview of physico-chemical properties for PFOA isomer 2,2,3,3,5,5,6,6,6-nonafluoro-4,4-bis(trifluoromethyl)-hexanoic acid, CAS Number 1192593-79-5.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa		
Melting/freezing point		
Boiling point at 760 Torr	158.5 ± 35.0°C	Calculated [a]
Vapour pressure at 25°C	183 Pa	Calculated [a]
Water solubility at pH = 7 and 25°C	4.1 g/L, 0.010 mol/L	Calculated [a]
Partition coefficient n-octanol/water (log value)	4.06 at pH = 7 and 25°C 5.59	Calculated [a] EPI [b]
Dissociation constant at 25°C	pKa = 0.42 ± 0.10	Calculated [a]

[a] From CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

[#] SMILES: O=C(O)C(F)(F)C(F)(F)C(C(F)(F)(F))(C(F)(F)(F))C(F)(F)C(F)(F)F

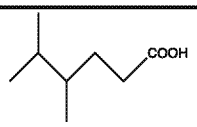
1.1.9 CAS Registry Number 1144512-36-6

No commercial sources are listed in CAS for PFOA isomer 2,2,3,3,4,5,6,6,6-nonafluoro-4,5-bis(trifluoromethyl)-hexanoic acid[#] (CAS Registry Number 1144512-36-6).

The references listed in CAS refer to a toxicology study [*Benskin et al.*, 2009], and to a conference contribution describing analysis of LC/ESI-MS/MS spectra of a series of PFOA isomers [*Arsenault et al.*, 2008].

There are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.10** summarises theoretical data listed in CAS.

Table 1.10. Overview of physico-chemical properties for PFOA isomer 2,2,3,3,4,5,6,6,6-nonafluoro-4,5-bis(trifluoromethyl)-hexanoic acid, CAS Number 1144512-36-6.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa		
Melting/freezing point		
Boiling point at 760 Torr	167.9 ± 35.0°C	Calculated [a]
Vapour pressure at 25°C	110 Pa	Calculated [a]
Water solubility at pH = 7 and 25°C	6.6 g/L, 0.016 mol/L	Calculated [a]
Partition coefficient n-octanol/water (log value)	3.50 at pH = 7 and 25°C 4.89	Calculated [a] EPI [b]
Dissociation constant at 25°C	pKa = 0.45 ± 0.10	Calculated [a]

[a] From CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

[#] SMILES: O=C(O)C(F)(F)C(F)(F)C(C(F)(F)(F))(F)C(F)(C(F)(F)(F))C(F)(F)F

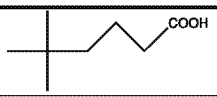
1.1.10 CAS Registry Number 1144512-34-4

No commercial sources are listed in CAS for PFOA isomer 2,2,3,3,4,4,6,6,6-nonafluoro-5,5-bis(trifluoromethyl)-hexanoic acid[#] (CAS Registry Number 1144512-34-4).

The references listed in CAS refer to a toxicology study [*Benskin et al.*, 2009], and to a conference contribution describing analysis of LC/ESI-MS/MS spectra of a series of PFOA isomers [*Arsenault et al.*, 2008].

There are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.11** summarises theoretical data listed in CAS.

Table 1.11. Overview of physico-chemical properties for PFOA isomer 2,2,3,3,4,4,6,6,6-nonafluoro-5,5-bis(trifluoromethyl)-hexanoic acid, CAS Number 1144512-34-4.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa		
Melting/freezing point		
Boiling point	150.8 ± 35.0	Calculated [a]
Vapour pressure at 25°C	273 Pa	Calculated [a]
Water solubility at pH = 7 and 25°C	11 g/L; 0.027 mol/L	Calculated [a]
Partition coefficient n-octanol/water (log value)	2.88 at pH = 7 and 25°C 5.59	Calculated [a] EPI [b]
Dissociation constant at 25°C	pK_a = 0.52 ± 0.10	Calculated [a]

[a] From CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

[#] SMILES: O=C(O)C(F)(F)C(F)(F)C(F)(F)C(C(F)(F)(F))(C(F)(F)(F))C(F)(F)F

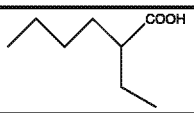
1.1.11 CAS Registry Number 35605-76-6

No commercial sources are listed in CAS for PFOA isomer 2,3,3,4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid[#] (CAS Registry Number 35605-76-6).

The references listed in CAS refer to preparative work [*Gambaretto et al.*, 1971], and to patents [*Gajewski*, 1986; *W-Q Fan and Manzara*, 1998; *Manzara et al.*, 1998; *Stern and Fan*, 1998; *Kawaguchi et al.*, 2009].

There are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.12** summarises theoretical data listed in CAS.

Table 1.12. Overview of physico-chemical properties for PFOA isomer 2,3,3,4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid, CAS Number 35605-76-6.

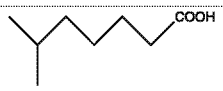
Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa		
Melting/freezing point		
Boiling point	150.8 ± 35.0	Calculated [a]
Vapour pressure at 25°C	273 Pa	Calculated [a]
Water solubility at pH = 7 and 25°C	11 g/L; 0.027 mol/L	Calculated [a]
Partition coefficient n-octanol/water (log value)	3.43 at pH = 7 and 25°C 5.59	Calculated [a] EPI [b]
Dissociation constant at 25°C	pK_a = 0.52 ± 0.10	Calculated [a]

[a] From CAS. Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs). [b] From the EPI suite [*Syracuse_Research_Corporation*, 2000-2008].

[#] SMILES: O=C(O)C(F)(C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

1.1.12 Summary of physico-chemical data for PFOA and PFOA isomers

Melting points and boiling points are available for PFOA and one PFOA isomer (2,2,3,3,4,4,5,5,6,6,7,7, 8,8,8-pentadecafluoro-octanoic acid and 2,2,3,3,4,4,5,5,6,7,7,7-dodecafluoro-6-(trifluoromethyl)-heptanoic acid):

	m.p. 54.9-55.6 °C b.p. 189 °C	[*Hare et al.*, 1954] [*Kauck and Diesslin*, 1951]
	m.p. 13-14 °C b.p. 189 °C	[Shinoda et al., 1972] *Wroblewska et al.*, 2006]

The calculated boiling point of the branched PFOA is 20 °C lower than the measured value suggesting that the results from model calculations should not be over interpreted.

The PFOA **vapour pressure** measurements all show a vapour pressure of around 4 Pa at 25 °C [*Kaiser et al.*, 2005; *Washburn et al.*, 2005; *Barton et al.*, 2008]. The Advanced Chemistry Development Software from ACD Labs[#] predicts vapour pressures of PFOA and various PFOA isomers from 37 to 273 Pa. Vapour pressure predictions from the EPI suite [*Syracuse_Research_Corporation*, 2000-2008] appear more reasonable and vary between 19 and 35 Pa. The vapour pressure of PFOA depends on temperature and can be calculated from [*Barton et al.*, 2008]:

$$\ln\left(p/\mathrm{Pa}\right) = \frac{-10695}{T} + 37.292$$

Concerning **the acid strength** of PFOA, there is a major discrepancy between experimental [*Brace*, 1962; *Radell et al.*, 1965; *Burns et al.*, 2008] and theoretical estimates [*Goss*, 2008]. The experimental data are all obtained from titration of aqueous solutions of ethanol or methanol, and are subject to empiric corrections. The work of Goss et al. [2008] is based on comparisons between experimental values for pK_a's of CF_3COOH and other acids (CHF_2COOH, CH_2FCOOH, CF_3CH_2COOH and $CF_3CH_2CH_2COOH$), and predictions from the QSAR program SPARC [*Hilal et al.*, 1995] and the quantum chemistry based estimation program COSMOS-RS [*Klamt*, 2005]. The latter method predicts the same pK_a values for CF_3COOH and PFOA and this is used as argument that these two acids should have the same acid strengths. The Advanced Chemistry Development Software from ACD Labs[#] predicts that the acid strengths of PFOA and the (branched) PFOA isomers have pKa values ranging from -0.47 to 0.52.

Fan et al. [1988] carried out a series of titration experiments to establish the strength of perfluorocarboxylic acids. 10^{-4} M solutions were potentiometrically titrated with NaOH. The Figure to the right is taken from their publication and shows that data for n-perfluorodecanoic acid agree with those obtained for nitric acid suggesting its complete dissociation. Similar results were obtained with $C_7F_{15}COOH$ and C_3F_7COOH. It should be noticed that no acid strengths were extracted from the experiments.

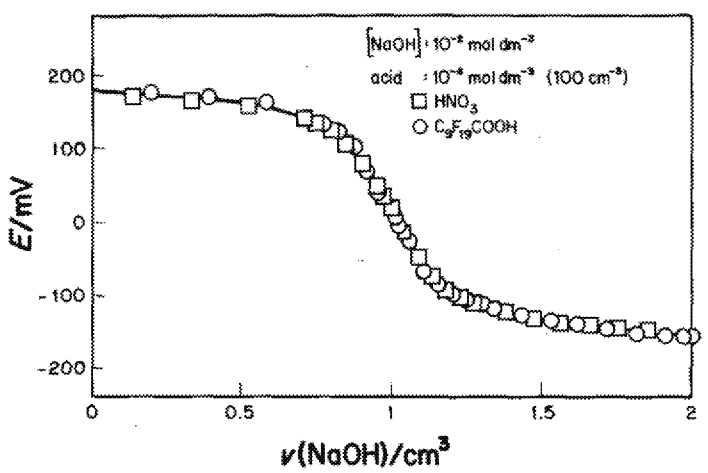


Fig. 1. Potentiometric titration of perfluorodecanoic (○) and nitric (□) acids at 25 °C. Cell: glass electrode – Ag/AgCl reference electrode

[#] http://www.acdlabs.com/home/

Recent experimental results for the dissociation constants of CF_3CF_2COOH ($K_a = 2.5\times10^{-2}$, $pK_a = 1.6$) and $CF_3CF_2CF_2COOH$ ($K_a = 1.58\times10^{-2}$, $pK_a = 1.8$) in water [*Chechina et al.*, 2007] suggest that conclusions of Goss et al. [2008] are questionable, and that the acid strength of PFOA and branched PFOA isomers will be somewhere between $pK_a = 1.8$ and 2.8.

The partitioning of PFOA in the environment strongly depends on its acid strength. This is reflected in the ratio between anionic and neutral forms of PFOA in aqueous solution. This ratio can easily be estimated assuming activity coefficients of unity:

$$\frac{[CF_3(CF_2)_6COO^-]}{[CF_3(CF_2)_6COOH]} = 10^{-pKa}\times10^{pH} =$$

pKa	$pH=4$	$pH=5$	$pH=6$
−0.5	3.16×10^{4}	3.16×10^{5}	3.16×10^{6}
2.8	1.58×10^{1}	1.58×10^{2}	1.58×10^{3}
3.5	3.16	3.16×10^{1}	3.16×10^{2}

Assuming a pK_a of 2.8, more than 99% of aqueous PFOA exists as its anionic form, which will not partition into the gas phase, at typical environmental pH of 5–8. However, since the Henrys Law constant, K_H, of PFOA is relatively small at 298 K (9.9 mol dm^{-3} for $pK_a = 2.8$), the partitioning of PFOA in air is possible. Kutsuna and Hori [2008] illustrates this for a rain cloud with 10^{-4} dm^3 water per 10^2 dm^3 of air and a pH value of 5 at 298 K: 96% of PFOA would partition into the air. Should pK_a be less than 2.8, less PFOA would partition into the air under the same atmospheric condition.

There is an obvious discrepancy between observations and theoretical predictions of acid strengths. It is very difficult to determine pK_a for PFOA experimentally, however available data supports that the acid strength of PFOA and branched PFOA isomers will be somewhere between $pK_a = 1.8$ and 2.8. If it turns out that higher accuracy of PFOA partitioning is needed in environmental impact assessment studies, a systematic theoretical study of PFCA and PFOA acid strengths could be undertaken.

Arp and Goss [2009] determined the gas/particle partitioning coefficient for PFOA and compared the results to model calculations. K_{ip}, is defined as:

$$K_{ip}\ (m^3/g) = c_{ip}/c_{iair}$$

where c_{ip} is the equilibrium concentration of compound "i" sorbed to the particle phase (mol_{ip}/g_p) and c_{iair} is the equilibrium concentration of *i* in the vapour phase (mol_i air/ m^3air). Their results suggest that dry aerosol sequestration is not an important atmospheric removal process for PFOA.

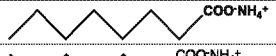
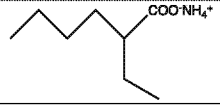
1.2 Physico-chemical data for (branched) pentadeca octanoic acid ammonia salt

The CAS Registry Number 90480-56-1 is a generic registration number that covers all branched pentadecafluoro octanoic acid ammonia salts (the number itself cannot be used for search in the CAS database). The European Inventory of Existing Commercial chemical Substances (EINECS) catalogues branched pentadeca octanoic acid ammonia salts under No. 291-791-3.

Of the 39 possible structural isomers of pentadecafluoro octanoic acid only 4,

Table 1.13, are registered in CAS with an ammonia salt.

Table 1.13. Summary of CAS Registry information on ammonium salts of PFOA isomers.

Chain length & Structure	CAS	Number of references
8 	3825-26-1	588 References
7 	207678-62-4	3 References
7 	19742-57-5	3 References
6 	13058-06-5	No references

1.2.1 CAS Registry Number 3825-26-1

There are numereous suppliers of the ammonium salt of the PFOA isomer 2,2,3,3,4,4,5,5,6,6, 7,7,8,8,8-pentadecafluoro-octanoic acid (CAS RN 3825-26-1. Deleted CAS RNs: 77751-76-9, 95328-99-7). Experimental physico-chemical data for the ammonium salt of n-pentadeca octanoic acid are summarized in **Table 1.14**, which also includes model results.

Table 1.14. Overview of physico-chemical properties for the ammonium salt of PFOA isomer 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-octanoic acid, CAS Number 3825-26-1.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting point	157-165 °C (decomposition starts above 105 °C)	[*Lines and Sutcliffe*, 1984]
Boiling point	decomposition	
Vapour pressure	<0.1 hPa at 20 °C 0.012 Pa at 25 °C 0.0028 Pa at 25 °C	MSDS [a] [*Washburn et al.*, 2005] [*Barton et al.*, 2009]
Water solubility at c.m.c. [b]	0.033 mol/L, 14.2 g/L at 2.5 °C	[*Shinoda et al.*, 1972]
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pKa for 	see section 1.1.1, page 8
pH value in water at 23 °C	5.4 at 20g/L	MSDS [a]

[a] Materials Safety Data Sheet, Sigma-Aldrich. [b] c.m.c, Critical micelle concentration.

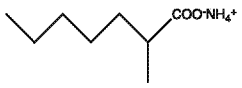
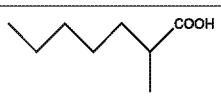
1.2.2 CAS Registry Number 207678-62-4

No commercial sources are listed in CAS for the ammonium salt of PFOA isomer 2,3,3,4,4,5,5,6,6, 7,7,7-dodecafluoro-2-(trifluoromethyl)-heptanoic acid (CAS Registry Number 207678-62-4).

The 3 references listed in CAS all relate to patent [*W-Q Fan and Manzara*, 1998; *Manzara et al.*, 1998; *Stern and Fan*, 1998].

Besides the calculated pK_a of the PFOA isomer (see page 9), there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.15** summarises available experimental and theoretical data listed in CAS.

Table 1.15. Overview of physico-chemical properties for the ammonium salt PFOA isomer 2,3,3,4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid, CAS Number 207678-62-4.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point		
Boiling point		
Vapour pressure		
Water solubility		
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	See section 1.1.2, page 9
pH value in water at 23 °C		

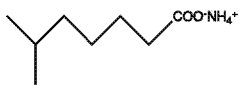
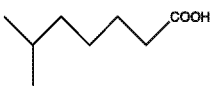
1.2.3 CAS Registry Number 19742-57-5

No commercial sources are listed in CAS for the ammonium salt of PFOA isomer 2,2,3,3,4,4,5,5,6, 7,7,7-dodecafluoro-6-(trifluoromethyl)-heptanoic acid (CAS Registry Number 19742-57-5).

The 3 references listed in CAS relate to patent [*Kometani et al.*, 1968], use [*Naonori and Koji*, 1985], and surface tension [*Blaszczak et al.*, 2001]. Besides the calculated pK_a of the PFOA isomer (see page 13), there are no relevant experimental physico-chemical data available in the literature for the compound.

Table 1.16 summarises available experimental and theoretical data listed in CAS.

Table 1.16. Overview of physico-chemical properties for the ammonium salt of PFOA isomer 2,3,3, 4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid, CAS Number 19742-57-5.

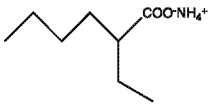
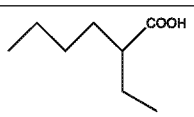
Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point		
Boiling point		
Vapour pressure		
Water solubility		
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	See section1.1.6, page 13
pH value in water at 23 °C		

1.2.4 CAS Registry Number 13058-06-5

No commercial sources are listed in CAS for the ammonium salt of PFOA isomer 2,3,3,4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid (CAS Registry Number 13058-06-5). There are no references listed in CAS.

Besides the calculated pK_a of the PFOA isomer (see page 18), there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.17** summarises available experimental and theoretical data listed in CAS.

Table 1.17. Overview of physico-chemical properties for the ammonium salt of PFOA isomer 2,3,3,4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid, CAS Number 13058-06-5.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point		
Boiling point		
Vapour pressure		
Water solubility		
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	See section 1.1.11, page 18
pH value in water at 23 °C		

1.2.5 Summary of physico-chemical data for ammonium salts of (branched) PFOA isomers

The **melting point** of APFO (the PFOA ammonium salt) is not accurately determined, m.p. 157-165 °C [*Lines and Sutcliffe*, 1984]. Figure 1.1 shows the weight loss during heating the salt. The study of Lines and Sutcliffe does not contain information about composition of the solid and gas phase during heating. It is likely that the compound starts to decompose around 105 °C, when NH_3 starts to evaporate from the salt (PFOA has a boiling point of 189 °C [*Kauck and Diesslin*, 1951]). It is expected that the branched PFOA ammonium salts will have very similar thermal stabilities.

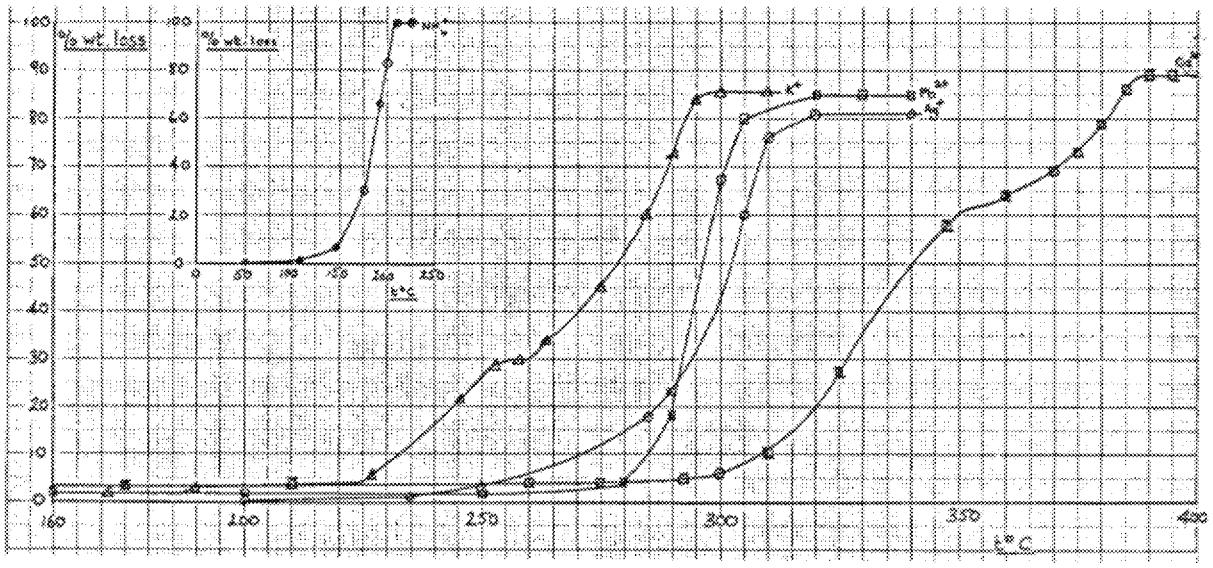


Figure 1.1. Thermogravemetric analysis of salts of perfluorooctanoic acid. From Lines and Sutcliffe, 1984.

The **thermal decomposition** of a number of salts of the straight chain perfluoro acids has been investigated [*LaZerte et al.*, 1953]. Only one ammonium salt was studied, $C_3F_7CO_2NH_4$, and this salt differs from the other butyrates in that the major fluorinated compound formed is $CF_3CF_2CF_2H$ – the other salts give perfluoro propene and/or carbonyl-containing compounds. It is expected that thermal decomposition of PFOA ammonium salts will decompose in a similar way resulting in $C_6F_{13}CF_2H + CO_2 + NH_3$.

The **solubility** of the PFOA ammonium salt is reported to be 0.033 mol/L at critical micelle concentration and 2.5 °C [*Shinoda et al.*, 1972]. This corresponds to around 14 g/L. The experimental data for PFOA isomer solubility are nearly identical (see section 1.1.12 page 19). Consequently, there cannot be large differences in the solubilities of branched PFOA ammonium salts.

The **vapour pressure** of APFO was measured in the range 90-165 °C [*Washburn et al.*, 2005], and the data fitted to the expression:

$$Log_{10}\left(p/mmHg\right) = -18.3324 + 502.464/T + 0.04231 \times T$$

from which the pressure at lower temperatures may be extrapolated. Considering that APFO is reported to decompose above 105 °C these vapour pressure data should be treated with caution.
The **vapour pressure** of APFO was also measured in the region 45-60 °C [*Barton et al.*, 2009], and the data fitted to the expression:

$$\ln\left(p/Pa\right) = \frac{-10936}{T} + 30.814$$

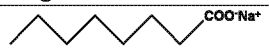
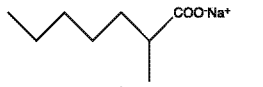
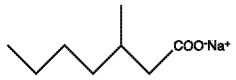
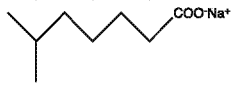
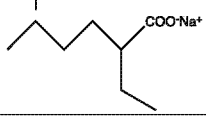
from which the pressure at lower temperatures may be extrapolated.

1.3 Physico-chemical data for (branched) pentadeca octanoic acid sodium salt

There is no generic identifier for all sodium salts of the various PFOA sodium salts in the CAS Registry. The European Inventory of Existing Commercial chemical Substances (EINECS) catalogues the PFOA sodium salt under No. 206-404-5.

Of the 39 possible structural isomers of pentadecafluoro octanoic acid only 4 are registered in CAS with a sodium salt, **Table 1.18**.

Table 1.18. Summary of CAS Registry information on sodium salts of PFOA isomers.

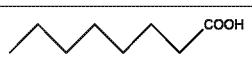
Chain length & Structure	CAS	Number of references
8 	335-95-5	325 References
7 	207678-72-6	3 References
7 	646-84-4	1 reference
7 	18017-22-6	7 References
6 	1195164-59-0	No references

1.3.1 CAS Registry Number 335-95-5

There are several suppliers of the sodium salt of the PFOA isomer 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-penta-decafluoro-octanoic acid (CAS Number 335-95-5).

There are around 325 references in CAS of which around 170 address substance properties. However, none of the references are relevant to an environmental impact assessment. Besides the calculated pK_a of the PFOA isomer (see page 8), there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.19** summarises the available information.

Table 1.19. Overview of physico-chemical properties for the sodium salt of PFOA isomer 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-octanoic acid, CAS Number 335-95-5.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point	~275 °C 273-275 °C (decomp. starts above 240 °C)	MSDS [a] [*Lines and Sutcliffe*, 1984]
Boiling point		
Vapour pressure		
Water solubility at c.m.c.[b]	0.036 mol/L at 8.0 °C	[*Shinoda et al.*, 1972]
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	See section 1.1.1, page 8
pH value in water at 23 °C		

[a] From Material Data Safety Sheet, Fluorochem. [b] c.m.c, Critical micelle concentration.

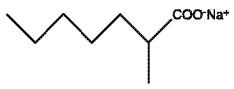
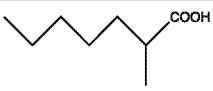
1.3.2 CAS Registry Number 207678-72-6

No commercial sources are listed in CAS for the sodium salt of PFOA isomer 2,3,3,4,4,5,5,6,6, 7,7,7-dodecafluoro-2-(trifluoromethyl)-heptanoic acid (CAS Registry Number 207678-72-6).

The 3 references listed in CAS relate to patent and do not contain data relevant to the present study [*W-Q Fan and Manzara*, 1998; *Manzara et al.*, 1998; *Stern and Fan*, 1998].

Besides the calculated pK_a of the PFOA isomer (see page 9), there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.20** summarises available experimental and theoretical data listed in CAS.

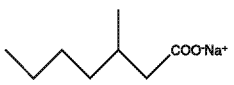
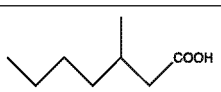
Table 1.20. Overview of physico-chemical properties for the sodium salt PFOA isomer 2,3,3, 4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid, CAS Number 207678-72-6.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point		
Boiling point		
Vapour pressure		
Water solubility		
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	See section 1.1.2, page 9
pH value in water at 23 °C		

1.3.3 CAS Registry Number 646-84-4

The reference listed in CAS relates to patent and does not contain data relevant to the present study [*Pennsalt Chemicals Corp*, 1963].

Table 1.21. Overview of physico-chemical properties for the sodium salt of PFOA isomer 2,2,3,4,4,5,5,6,6,7,7,7-dodecafluoro-3-(trifluoromethyl)-heptanoic acid, CAS Number 646-84-4.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point		
Boiling point		
Vapour pressure		
Water solubility		
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	See section 1.1.3, page 10
pH value in water at 23 °C		

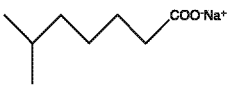
1.3.4 CAS Registry Number 18017-22-6

No commercial sources are listed in CAS for the sodium salt of PFOA isomer 2,2,3,3,4,4,5,5,6, 7,7,7-dodecafluoro-6-(trifluoromethyl)-heptanoic acid (CAS Registry Number 18017-22-6).

Three of the 7 references listed in CAS relate to patent and do not contain data relevant to the present study [*Daikin Kogyo Co Ltd*, 1966; 1973; *Katsushima et al.*, 1976]. The other references deal with surface activity of PFOA sodium salts [*Meissner et al.*, 1992; *Meissner et al.*, 2006], and with solubility and micelle formation [*Hato and Shinoda*, 1970; *Shinoda et al.*, 1972].

Besides the calculated pK_a of the PFOA isomer (see page 13), there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.22** summarises available experimental and theoretical data listed in CAS.

Table 1.22. Overview of physico-chemical properties for the sodium salt of PFOA isomer 2,3,3,4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid, CAS Number 18017-22-6.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point		
Boiling point		
Vapour pressure		
Water solubility at c.m.c.[a]	0.032 mol/L at 25 °C	[*Shinoda et al.*, 1972]
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	see section 1.1.6, page 13
pH value in water at 23 °C		

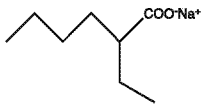
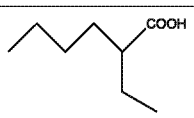
[a] c.m.c, Critical micelle concentration

1.3.5 CAS Registry Number 1195164-59-0

No commercial sources are listed in CAS for the sodium salt of PFOA isomer 2,3,3,4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid (CAS Registry Number 18017-22-6).

Besides the calculated pK_a of the PFOA isomer (see page18), there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.23** summarises available experimental and theoretical data listed in CAS.

Table 1.23. Overview of physico-chemical properties for the sodium salt of PFOA isomer 2,3,3,4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid, CAS Number 1195164-59-0.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point		
Boiling point		
Vapour pressure		
Water solubility		
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	see section 1.1.11, page 18
pH value in water at 23 °C		

1.3.6 Summary of physico-chemical data for sodium salts of branched PFOA isomers

The **melting point** of the PFOA sodium salt is determined to be 273-275 °C [*Lines and Sutcliffe*, 1984]. Figure 1.2 shows the weight loss during heating the salt. The study of Lines and Sutcliffe does not contain information about composition of the solid and gas phase during heating. It is likely that the compound starts to decompose already around 240 °C resulting in NaF formation. It is expected that the branched PFOA sodium salts will have very similar thermal stabilities.

The **thermal decomposition** of sodium salts of the straight chain perfluoro acids has been shown to result in perfluoroalkenes, CO_2 and NaF [*Haszeldine*, 1952]: $CF_3(CF_2)_nCF_2CF_2CO_2Na \rightarrow CF_3(CF_2)_nCF=CF_2 + CO_2 + NaF$. It is expected that branched PFOA sodium salts will undergo similar thermal decomposition.

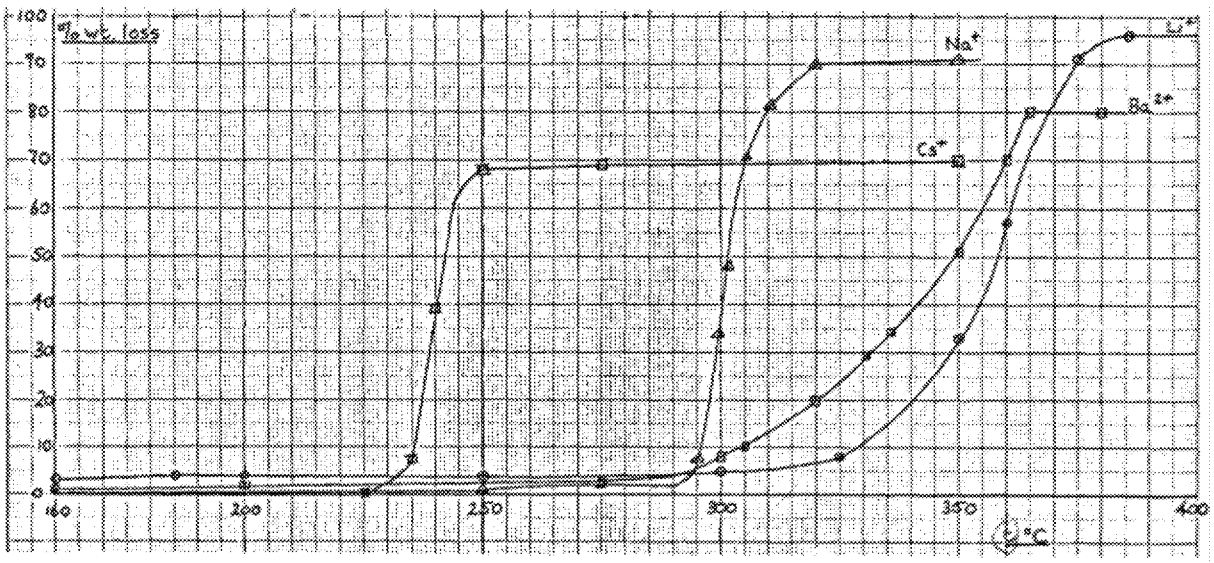


Figure 1.2. Thermogravemetric analysis of salts of perfluorooctanoic acid. From Lines and Sutcliffe, 1984.

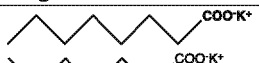
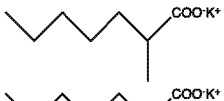
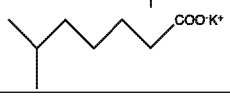
The **solubility** of the PFOA sodium salt is reported to be 0.036 mol/L at critical micelle concentration and 8.0 °C [*Shinoda et al.*, 1972]. This corresponds to around 16 g/L. The experimental data for PFOA isomer solubility are nearly identical (see section 1.1.12 page 19). Consequently, there cannot be large differences in the solubilities of branched PFOA sodium salts.

1.4 Physico-chemical data for (branched) pentadeca octanoic acid potassium salt

There is no generic identifier for all potassium salts of the various PFOA potassium salts in the CAS Registry. The European Inventory of Existing Commercial chemical Substances (EINECS) catalogues the PFOA potassium salt under No. 219-248-8.

Of the 39 possible structural isomers of pentadecafluoro octanoic acid only 3 are registered in CAS with a potassium salt, **Table 1.24**.

Table 1.24. Summary of CAS Registry information on potassium salts of PFOA isomers.

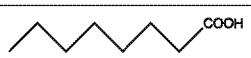
Chain length & Structure	CAS	Number of references
8 	2395-00-8	80 References
7 	207678-65-7	2 References
7 	29457-73-6	3 References

1.4.1 CAS Registry Number 2395-00-8

There are several suppliers of the potassium salt of the PFOA isomer 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-octanoic acid (CAS Number 2395-00-8).

Besides the calculated pK_a of the PFOA isomer (see page 8), there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.25** summarises available experimental and theoretical data listed in CAS.

Table 1.25. Overview of physico-chemical properties for the potassium salt of PFOA isomer 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-octanoic acid, CAS Number 2395-00-8.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point	222-235 °C (decomp. Starts at 225 °C)	[*Lines and Sutcliffe*, 1984]
Boiling point		
Vapour pressure		
Water solubility at c.m.c.[a]	0.027 mol/L at 25.6 °C	[*Shinoda et al.*, 1972]
Water solubility (-log K at 25 °C)	3.59 ± 0.26	[*X J Fan et al.*, 1988]
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	See section 1.1.1, page 8
pH value in water at 23 °C		

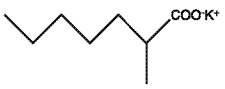
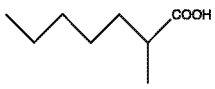
[a] c.m.c, Critical micelle concentration.

1.4.2 CAS Registry Number 207678-65-7

No commercial sources are listed in CAS for the potassium salt of PFOA isomer 2,3,3,4,4,5,5,6,6, 7,7,7-dodecafluoro-2-(trifluoromethyl)-heptanoic acid (CAS Registry Number 207678-65-7).

Besides the calculated pK_a of the PFOA isomer (see page 9), there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.26** summarises available experimental and theoretical data listed in CAS.

Table 1.26. Overview of physico-chemical properties for the potassium salt PFOA isomer 2,3,3, 4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid, CAS Number 207678-65-7.

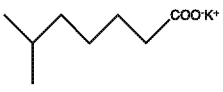
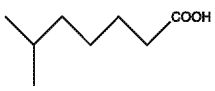
Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point		
Boiling point		
Vapour pressure		
Water solubility		
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	See section 1.1.2, page 9
pH value in water at 23 °C		

1.4.3 CAS Registry Number 29457-73-6

No commercial sources are listed in CAS for the potassium salt of PFOA isomer 2,2,3,3,4,4,5,5,6, 7,7,7-dodecafluoro-6-(trifluoromethyl)-heptanoic acid (CAS Registry Number 29457-73-6).

Besides the calculated pK_a of the PFOA isomer (see page 13), there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.27** summarises available experimental and theoretical data listed in CAS.

Table 1.27. Overview of physico-chemical properties for the potassium salt of PFOA isomer 2,3,3, 4,4,5,5,6,6,6-decafluoro-2-(1,1,2,2,2-pentafluoroethyl)-hexanoic acid, CAS Number 29457-73-6.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point		
Boiling point		
Vapour pressure		
Water solubility at c.m.c.[a]	0.030 mol/L at 25 °C	[*Shinoda et al.*, 1972]
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	see section 1.1.6, page 13
pH value in water at 23 °C		

1.4.4 Summary of physico-chemical data for potassium salts of branched PFOA isomers

The **melting point** of the PFOA potassium salt is not accurately determined, m.p. 222-235 °C [*Lines and Sutcliffe*, 1984]. Figure 1.1 (page 26) shows the weight loss during heating the salt. The study of Lines and Sutcliffe does not contain information about composition of the solid and gas phase during heating. It is likely that the compound starts to decompose around 225 °C resulting in KF formation.

LaZerte and co-workers studied the **thermal decomposition** of a potassium perfluorobutyrate, $CF_3CF_2CF_2CO_2K$ [*LaZerte et al.*, 1953]. The salt decomposes to $CF_3CF{=}CF_2 + CO_2 + KF$ with a 98% yield. It is expected that thermal decomposition of PFOA potassium salts will result in similar products. It is also expected that the branched PFOA potassium salts will show similar thermal stabilities.

The **solubility** of the PFOA potassium salt is reported to be 0.027 mol/L at critical micelle concentration and 26.6 °C [*Shinoda et al.*, 1972]. This corresponds to around 12 g/L. The thermodynamic measurements by Fan et al. [1988] give a slightly lower solubility of 0.016 mol/L (assuming activity coefficients of 1). The experimental data for PFOA isomer solubility are nearly identical (see section 1.1.12 page 19). Consequently, there cannot be large differences in the solubilities of branched PFOA potassium salts.

1.5 Physico-chemical data for pentadeca octanoic acid silver salt

There is no generic identifier for all silver salts of the various PFOA silver salts in the CAS Registry. The European Inventory of Existing Commercial chemical Substances (EINECS) catalogues the PFOA silver salt under No. 206-402-4. There is only one PFOA silver salt in the CAS Register: 335-93-3.

1.5.1 CAS Registry Number 335-93-3

There are several suppliers of the silver salt of the PFOA isomer 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-penta-decafluoro-octanoic acid (CAS Number 335-93-3).

There are 23 references in CAS of which 4 address substance properties. However, none of the references are relevant to an environmental impact assessment. Besides the calculated pK_a of the PFOA isomer (see page 8), there are no relevant experimental physico-chemical data available in the literature for the compound. **Table 1.28** summarises the available information.

Table 1.28. Overview of physico-chemical properties for the potassium salt of PFOA isomer 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-octanoic acid, CAS Number 335-93-3.

Property	Value	Remarks
Structure		
Physical state at 20°C and 101.3 kPa	solid	
Melting/freezing point	220-225 °C (decomp. starts at 200 °C)	[*Lines and Sutcliffe*, 1984]
Boiling point		
Vapour pressure		
Water solubility (-log K at 25 °C)	5.02 ± 0.04	[*X J Fan et al.*, 1988]
Partition coefficient n-octanol/water (log value)		
Dissociation constant	pK_a for 	See section 1.1.1, page 8
pH value in water at 23 °C		

The **melting point** of the PFOA silver salt is not accurately determined, m.p. 220-235 ˚C [*Lines and Sutcliffe*, 1984]. Figure 1.1 (page 26) shows the weight loss during heating the salt. The study of Lines and Sutcliffe does not contain information about composition of the solid and gas phase during heating. It is likely that the compound starts to decompose around 200 ˚C resulting in AgF formation.

LaZerte and co-workers studied the **thermal decomposition** of a silver perfluorobutyrate and silver PFOA, [*LaZerte et al.*, 1953]. The salts decompose with 45% yield to C_6F_{14} and $C_{14}F_{30}$, respectively.

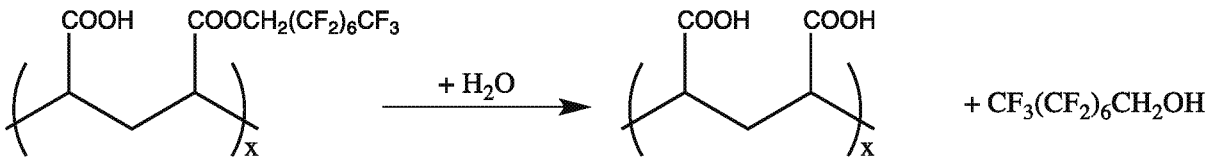
The **solubility** of the PFOA silver salt can be estimated from the thermodynamic measurements by Fan et al. [1988] gives a slightly lower solubility of 0.003 mol/L (assuming activity coefficients of 1). This corresponds to around 1.6 g/L. Consequently, the PFOA silver salt will be dissolved in water.

2 Potential PFOA Precursors

Table A.1 (ANNEX, page 52) presents a list of relevant PFOA precursors (from Environment Canada). Structure details of the listed precursors and comments related to their degradation are presented in the following sections.

2.1 2-Propenoic acid, 2-methyl-, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl ester, polymer with 2-propenoic acid

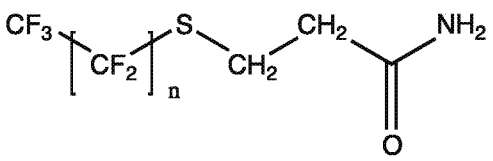
This co-polymer (CAS RN 53515-73-4) contains (ester) side-chains >C-C(O)$OCH_2(CF_2)_6CF_3$ and may in principle undergo hydrolysis to give 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-1-octanol (CAS RN 307-30-2).



Aqueous phase photo-oxidation of $CF_3(CF_2)_6CH_2OH$ will result in PFOA. Gas phase photo-oxidation will lead to $CF_3(CF_2)_6CHO$ and subsequently in part to PFOA [*Wallington et al.*, 2006].

2.2 3-[(γ-ω-perfluoro-C_{4-10}-alkyl)thio] Propanamide derivatives

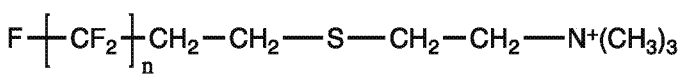
The CAS RN 68187-42-8 is a generic identifier and cannot be used for searching the CAS Registry. The European Inventory of Existing Commercial chemical Substances (EINECS) catalogues the polymer under No.269-095-6 .



This class of compounds are not PFOA precursors – degradation will likely lead to $CF_3(CF_2)_nSO_3H$.

2.3 α-fluoro-ω-[2- [[2-(trimethylammonio)ethyl]thio]ethyl]-poly(difluoromethylene) methyl sulfate

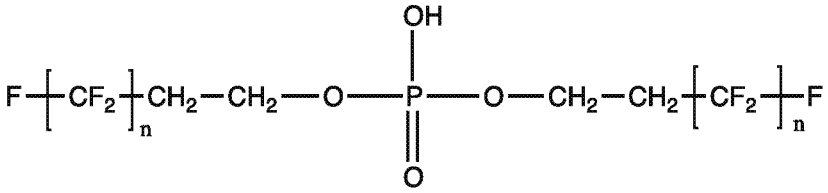
The compound (CAS RN 65530-57-6) is a salt of $CH_3OSO_3^-$ with the trimethylamine:



Degradation will lead to $F(CF_2)_nCOOH$ (PFOA for n=7).

2.4 α,α'-[phosphinicobis(oxy-2,1-ethanediyl)]bis[ω-fluoro-poly(difluoromethylene)

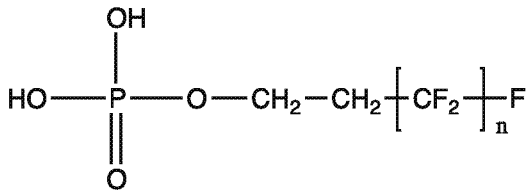
The compound (CAS RN 65530-62-3) is a phosphoric acid ester:



The phosphoric acid ester may in principle undergo hydrolysis and/or photo-oxidation eventually leading to $CF_3(CF_2)_{n-1}CHO$ (intermediate) and subsequently to $CF_3(CF_2)_{n-1}COOH$ (PFOA for n=7).

2.5 α-fluoro-ω-[2-(phosphonooxy)ethyl]-poly(difluoromethylene)

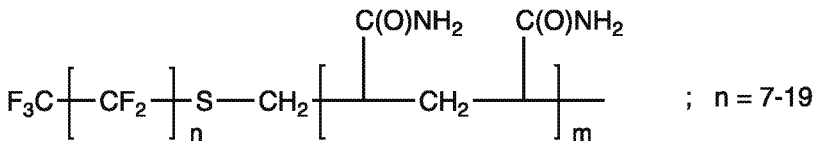
The compound (CAS RN 65530-61-2) is a phosphoric acid ester:



The phosphoric acid ester may in principle undergo hydrolysis and/or photo-oxidation eventually leading to $CF_3(CF_2)_{n-1}CHO$ (intermediate) and subsequently to $CF_3(CF_2)_{n-1}COOH$ (PFOA for n=7)

2.6 Thiols, C_{8-20}, γ-ω-perfluoro, telomers with acrylamide

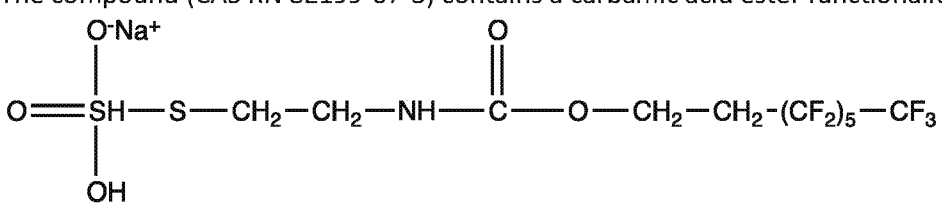
The acrylamide polymerisation is initiated by addition of the $CF_3(CF_2)_nS\cdot$ radical to CC double bond of acrylamide resulting in a polymer with the following structure (CAS RN 70969-47-0):



The compounds are not PFOA precursors. Degradation will likely lead to $CF_3(CF_2)_nSO_3H$.

2.7 C-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) [2-(sulfothio)ethyl]-carbamic acid ester, monosodium salt

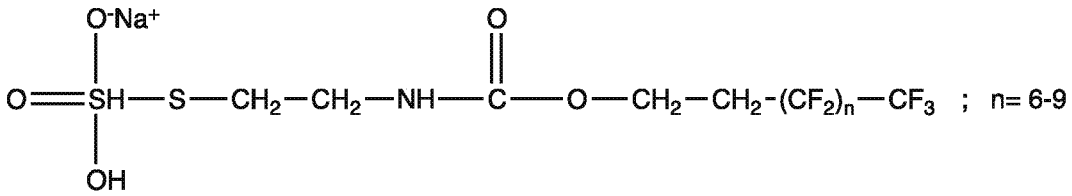
The compound (CAS RN 82199-07-3) contains a carbamic acid ester functionality:



The carbamic acid ester may in principle hydrolyse giving $CF_3(CF_2)_5CH_2CH_2OH$, which is a PFCA precursor and not a PFOA precursor.

2.8 C-(γ-ω-perfluoro-C_{6-9}-alkyl) [2-(sulphothio)ethyl]-carbamic acid esters, monosodium salts

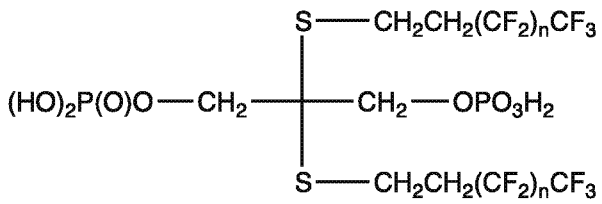
The compound (CAS RN 95370-51-7) contains a carbamic acid ester functionality:



The carbamic acid ester may in principle hydrolyse giving $CF_3(CF_2)_nCH_2CH_2OH$, which for n≥6 are PFOA precursors [*Wallington et al.*, 2006].

2.9 1,3-Propanediol, 2,2-bis[[(γ-ω-perfluoro-C_{4-10}-alkyl)thio]methyl] derivatives, phosphates, ammonium salts

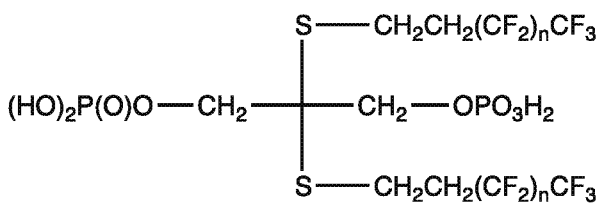
The substance (CAS RN 148240-85-1) contains $CF_3(CF_2)_nCH_2CH_2$-fragments (n=4-10) and has the general structure (ammonium not included):



Degradation will result in PFOA for n≥6.

2.10 1,3-Propanediol, 2,2-bis[[(γ-ω-perfluoro-C_{6-12}-alkyl)thio]methyl] derivatives, phosphates, ammonium salts

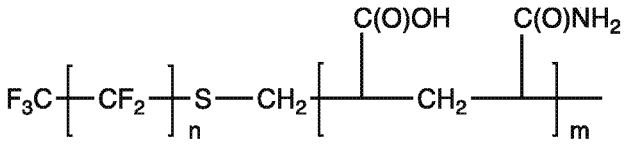
The substance (CAS RN 148240-87-3) contains $CF_3(CF_2)_nCH_2CH_2$-fragments (n=6-12) and has the general structure (ammonium not included):



Degradation will result in PFOA for n≥6.

2.11 Thiols, C_{4-20}, γ-ω-perfluoro, co-telomers with acrylic acid and acrylamide

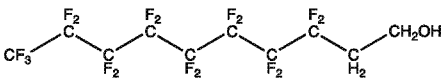
The substance will contain sub-structures like the following:



; n = 4-20

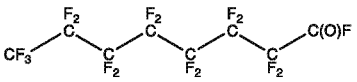
The substance is not a PFOA precursor. Degradation will likely result in $CF_3(CF_2)_nSO_3H$ and may therefore be a PFOS precursor for n=7.

2.12 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decanol

This compound has the following structure: 

Gas phase photo-oxidation of the $CF_3(CF_2)_7CH_2CH_2OH$ (CAS RN 678-39-7) will lead to $CF_3(CF_2)_7CHO$ and subsequently in part to PFOA [*Wallington et al.*, 2006].

2.13 Pentadecafluoro-octanoyl fluoride

This compound has the following structure: 

The acid fluoride (CAS RN 335-66-0) will undergo hydrolysis giving PFOA:

$CF_3(CF_2)_6C(O)F + H_2O \rightarrow CF_3(CF_2)_6C(O)O^- + HF + H^+$

2.14 Pentadecafluoro-octanoic acid methyl ester

The compound (CAS RN 376-27-2) is a PFOA precursor:

Photo-oxidation:

$CF_3(CF_2)_6C(O)OCH_3 + OH \rightarrow CF_3(CF_2)_6C(O)OCH_2 + H_2O$

$CF_3(CF_2)_6C(O)OCH_2 + O_2 \rightarrow CF_3(CF_2)_6C(O)OCH_2OO$

$CF_3(CF_2)_6C(O)OCH_2OO + NO \rightarrow CF_3(CF_2)_6C(O)OCH_2O + NO_2$

$CF_3(CF_2)_6C(O)OCH_2OO + ROO \rightarrow CF_3(CF_2)_6C(O)OCH_2O + RO + O_2$

$CF_3(CF_2)_6C(O)OCH_2OO + ROO \rightarrow \mathbf{CF_3(CF_2)_6C(O)OCH_2OH} + R'CHO + O_2$

$CF_3(CF_2)_6C(O)OCH_2OO + ROO \rightarrow \mathbf{CF_3(CF_2)_6C(O)OCHO} + R'CH_2OH + O_2$

$CF_3(CF_2)_6C(O)OCH_2O + O_2 \rightarrow \mathbf{CF_3(CF_2)_6C(O)OCHO} + HO_2$

Hydrolysis:

$CF_3(CF_2)_6C(O)OCH_3 + H_2O \rightarrow CF_3(CF_2)_6C(O)O^- + CH_3OH + H^+$

$\mathbf{CF_3(CF_2)_6C(O)OCHO} + H_2O \rightarrow CF_3(CF_2)_6C(O)O^- + HCOOH + H^+$

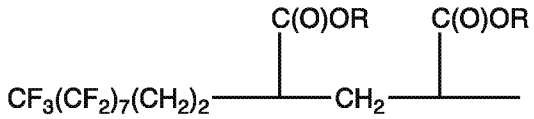
2.15 Pentadecafluoro-octanoic acid ethyl ester

The ester (CAS Registry Number 3108-24-5) is a PFOA precursor:

$CF_3(CF_2)_6C(O)OCH_2CH_3 + H_2O \rightarrow CF_3(CF_2)_6C(O)O^- + CH_3CH_2OH + H^+$

2.16 8:2 Fluorotelomer acrylate polymers

The substance will contain sub-structures like the following:



Degradation will therefore result in PFOA.

2.17 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-iododecane

The compound (CAS RN 2043-53-0) is a PFOA precursor. Iodides may undergo both photolysis and reactions with OH radicals in the troposphere and hydrolysis in water:

$CF_3(CF_2)_7CH_2CH_2I \xrightarrow{h\nu} CF_3(CF_2)_7CH_2CH_2 + I$

$CF_3(CF_2)_7CH_2CH_2 + O_2 \rightarrow CF_3(CF_2)_7CH_2CH_2OO$

$CF_3(CF_2)_7CH_2CH_2OO + NO \rightarrow CF_3(CF_2)_7CH_2CH_2O + NO_2$

$CF_3(CF_2)_7CH_2CH_2OO + ROO \rightarrow CF_3(CF_2)_7CH_2CH_2O + RO + O_2$

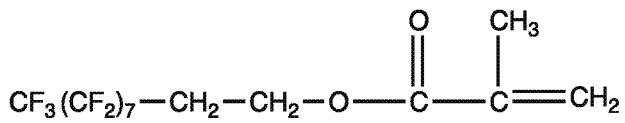
$CF_3(CF_2)_7CH_2CH_2OO + ROO \rightarrow \mathbf{CF_3(CF_2)_7CH_2CH_2OH} + R'CHO + O_2$

$CF_3(CF_2)_7CH_2CH_2OO + ROO \rightarrow \mathbf{CF_3(CF_2)_7CH_2CHO} + R'CH_2OH + O_2$

$CF_3(CF_2)_7CH_2CH_2O + O_2 \rightarrow \mathbf{CF_3(CF_2)_7CH_2CHO} + HO_2$

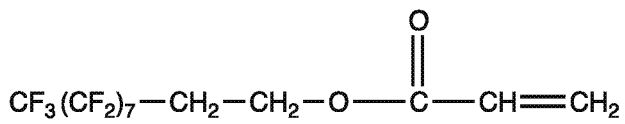
2.18 2-propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl methacrylate (C8-2 methacrylate)

The compound (CAS RN 1996-88-9) is an ester that may hydrolyse to $CF_3(CF_2)_7CH_2CH_2OH$ or undergo gas phase photo-oxidation to $CF_3(CF_2)_7CHO$. The compound is a PFOA precursor.



2.19 2-propenoic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl acrylate

The compound (CAS RN 27905-45-9) is an ester that may hydrolyse to $CF_3(CF_2)_7CH_2CH_2OH$ or undergo gas phase photo-oxidation to $CF_3(CF_2)_7CHO$. The compound is a PFOA precursor.



2.20 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodec-1-ene (C8-2 olefin)

The compound, $CF_3(CF_2)_7CH{=}CH_2$ (CAS RN 21652-58-4) will undergo gas phase or aqueous phase photo-oxidation to $CF_3(CF_2)_7CHO$, which is a PFOA precursor [*Wallington et al.*, 2006]. The gas phase reactions are expected to include (see also above):

$CF_3(CF_2)_7CH{=}CH_2 + OH \rightarrow CF_3(CF_2)_7CHOHCH_2 + H_2O$

$CF_3(CF_2)_7CHOHCH_2 + O_2 \rightarrow CF_3(CF_2)_7CHOHCH_2OO$

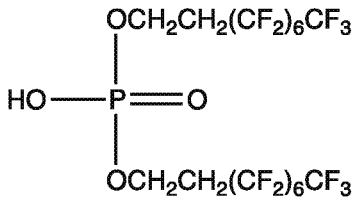
$CF_3(CF_2)_7CHOHCH_2OO + NO \rightarrow CF_3(CF_2)_7CHOHCH_2O + NO_2$

$CF_3(CF_2)_7CHOHCH_2O \xrightarrow{\Delta} CF_3(CF_2)_7CHOH + CH_2O$

$CF_3(CF_2)_7CHOH + O_2 \rightarrow \mathbf{CF_3(CF_2)_7CHO} + HO_2$

2.21 Phosphoric acid surfactants

Compounds such as 8:2 polyfluoroalkyl phosphoric acid diester or 8:2 diPAP



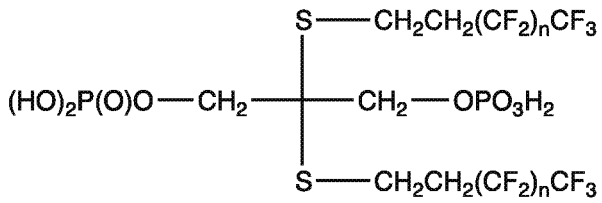
Degradation of these compounds will result in PFOA.

2.22 Perfluorooctylsulfonamides

Perfluorooctylsulfonamides have the general structure: $CF_3(CF_2)_7$-SO_2-NR_1R_2. This class of compounds are likely PFOS precursors and not PFOA precursors.

2.23 1,3-Propanediol, 2,2-bis[[(γ-ω-perfluoro-C10-20-alkyl)thio]methyl] derivs., phosphates, ammonium salts

The substance (CAS RN 148240-89-5) contains $CF_3(CF_2)_nCH_2CH_2$-fragments (n=10-20) and has the general structure (ammonium ion not included):



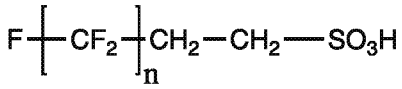
Degradation will result in C10 - C20 PFCAs.

2.24 Oxirane, methyl-, polymer with oxirane, mono[2-hydroxy-3-[(γ-ω-perfluoro-C8-20-alkyl)thio]propyl] ethers

This class of polymers (CAS RN 183146-60-3) contains $F(CF_2)_n$-S-$CH_2CHOHCH_2$-O-R. Degradation will likely result in compounds such as $F(CF_2)_n$-SO_3H and these ethers are not PFOA precursors.

2.25 α-fluoro-ω-(2-sulfoethyl)-poly(difluoromethylene)

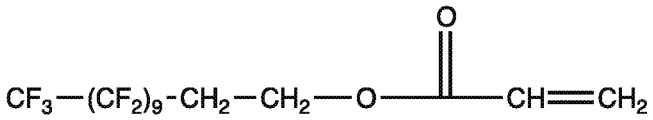
This class of compounds (CAS RN 80010-37-3) has the following chain structure and is a PFOA precursor for n≥7.



2.26 2-Propenoic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl ester, polymer with 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl 2-propenoate, alpha-(2-methyl-1-1-oxo-2-2-propenyl)-omega-[(2-methyl-1-oxo-2-propenyl)oxy]poly(oxy-1, 2-ethanediyl), 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-nonacosafluorohexadecyl 2-propenoate, octadecyl 2-propenoate, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl 2-propenoate and 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,18,18-tritriacontafluorooctadecyl 2-propenoate

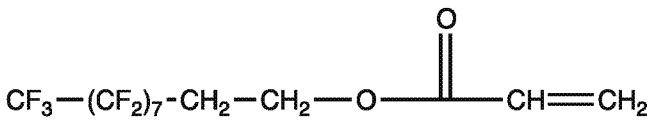
This co-polymer (CAS RN 116984-14-6) is made of the following mix of compounds:

1. 2-Propenoic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl ester (CAS RN 17741-60-5):



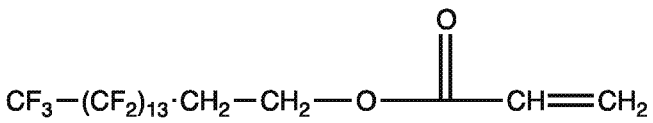
This is a PFCA precursor, and to some extend also a PFOA precursor [*Wallington et al.*, 2006].

2. 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl 2-propenoate (CAS RN 27905-45-9):



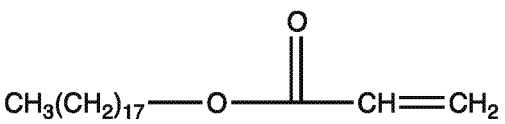
This is a PFCA precursor, and to some extend also a PFOA precursor [*Wallington et al.*, 2006].

3. 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-nonacosafluorohexadecyl 2-propenoate (CAS RN 34362-49-7):



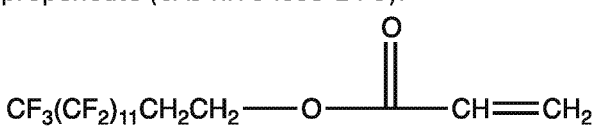
This is a PFCA precursor, and to some extend also a PFOA precursor [*Wallington et al.*, 2006].

4. octadecyl 2-propenoate (CAS RN 4813-57-4):



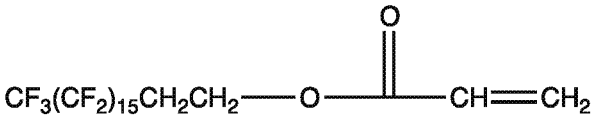
This sub-structure is not fluorinated.

5. 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl 2-propenoate (CAS RN 34395-24-9):



This is a PFCA precursor, and to some extend also a PFOA precursor [*Wallington et al.*, 2006].

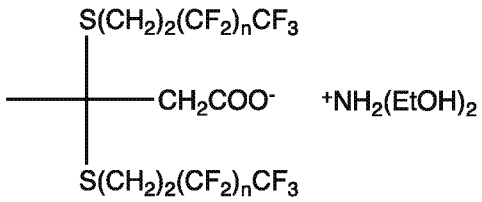
6. 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,18,18-tritriaconta-fluorooctadecyl 2-propenoate (CAS RN 65150-93-8):



This is a PFCA precursor, and to some extent also a PFOA precursor [*Wallington et al.*, 2006].

2.27 Pentanoic acid, 4,4-bis[(γ-ω-perfluoro-C8-20-alkyl)thio]derivs., compds. with diethanolamine

The substance (CAS RN 71608-61-2) contains $CF_3(CF_2)_nCH_2CH_2$-fragments (n=8-20) and has the general structure:



Degradation may result in C9 - C21 PFCAs. If these PFCAs are transferred to the gas phase they may undergo photo-oxidation and, to some extent, give PFOA [*Wallington et al.*, 2006].

3 Literature

Arp, H. P. H., and Goss, K.-U. (2009), Gas/Particle Partitioning Behavior of Perfluorocarboxylic Acids with Terrestrial Aerosols, *Environmental Science & Technology*, *43*(22), 8542-8547.

Arsenault, G., Chittim, B., McAlees, A., McCrindle, R., and Riddell, N. (2008), Analysis of perfluoroalkyl anion fragmentation pathways for branched perfluorooctanoic acids during LC/ESI-MS/MS, *Organohalogen Compd.*, *70*, 1329-1332.

Barton, C. A., Botelho, M. A., and Kaiser, M. A. (2008), Solid Vapor Pressure and Enthalpy of Sublimation for Perfluorooctanoic Acid, *J. Chem. Eng. Data*, *53*, 939-941.

Barton, C. A., Botelho, M. A., and Kaiser, M. A. (2009), Solid Vapor Pressure and Enthalpy of Sublimation for Ammonium Perfluorooctanoate, *J. Chem. Eng. Data*, *54*, 752-755.

Benskin, J. P., De, S. A. O., Martin, L. J., Arsenault, G., McCrindle, R., Riddell, N., Mabury, S. A., and Martin, J. W. (2009), Disposition of perfluorinated acid isomers in Sprague-Dawley rats; part 1: single dose, *Environ. Toxicol. Chem.*, *28*, 542-554.

Benskin, J. P., Ahrens, L., Muir, D. C. G., Scott, B. F., Spencer, C., Rosenberg, B., Tomy, G., Kylin, H., Lohmann, R., and Martin, J. W. (2012), Manufacturing Origin of Perfluorooctanoate (PFOA) in Atlantic and Canadian Arctic Seawater, *Environ. Sci. Technol.*, *46*, 677-685.

Bernett, M. K., and Zisman, W. A. (1959), Wetting of Low-Energy Solids by Aqueous Solutions of Highly Fluorinated Acids and Salts, *The Journal of Physical Chemistry*, *63*(11), 1911-1916.

Blaszczak, J., Sobcynska, A., Szymanowski, J., Twardochleb, B., and Meissner, E. (2001), Surface activity of surfactant mixtures containing fluorinated amphiphiles, *Tenside, Surfactants, Deterg.*, *38*, 368-372.

Brace, N. O. (1962), Long Chain Alkanoic and Alkenoic Acids with Perfluoroalkyl Terminal Segments1, *The Journal of Organic Chemistry*, *27*(12), 4491-4498.

Burns, D. C., Ellis, D. A., Li, H., McMurdo, C. J., and Webster, E. (2008), Experimental pK(a) Determination for Perfluorooctanoic Acid (PFOA) and the Potential Impact of pK(a) Concentration Dependence on Laboratory-Measured Partitioning Phenomena and Environmental Modeling, *Environmental Science & Technology*, *42*(24), 9283-9288.

Chechina, O. N., Sokolov, S. V., Berenblit, V. V., and Soshin, V. A. (2007), - *80*(- 10), - 1772.

Daikin Kogyo Co Ltd (1966), Water- and oil-resistant fluoroalkyl compositions for paper and fabrics, edited, p. 28 pp., Daikin Kogyo Co., Ltd. .

Daikin Kogyo Co Ltd (1967), ω,ω-Bis(trifluoromethyl)perfluorocarboxylic acids useful as surfactants and for manufacturing oil and water repellents, edited, p. 19 pp., Daikin Kogyo Co., Ltd.

Daikin Kogyo Co Ltd (1973), Fluorine-containing carboxylic acids, edited, p. 18 pp., Daikin Kogyo Co., Ltd. .

De Silva, A. O., Benskin, J. P., Martin, L. J., Arsenault, G., McCrindle, R., Riddell, N., Martin, J. W., and Mabury, S. A. (2009), Disposition of perfluorinated acid isomers in Sprague-Dawley rats; part 2: subchronic dose, *Environ. Toxicol. Chem.*, *28*, 555-567.

De Silva, A. O., Muir, D. C. G., and Mabury, S. A. (2009), Distribution of perfluorocarboxylate isomers in select samples from the North American environment, *Environ. Toxicol. Chem.*, *28*, 1801-1814.

Fan, W.-Q., and Manzara, A. P. (1998), Aqueous fluoropolymer compositions and their preparing methods, edited, p. 79 pp., Minnesota Mining and Manufacturing Co., USA .

Fan, X. J., Colic, M., Kallay, N., and Matijevic, E. (1988), Precipitation of surfactant salts. III. Metal perfluoroalkanecarboxylates, *Colloid Polym. Sci.*, *266*, 380-384.

Gajewski, R. P. (1986), Fluorinated alkanoyl anilides with biocidal activities, edited, p. 72 pp., Eli Lilly and Co., USA .

Gambaretto, G. P., Troilo, G., Napoli, M., and Fraccaro, C. (1971), Perfluorinated aliphatic α-alkyl-substituted acids. Preparation and mechanism of decarboxylation, *Chim. Ind. (Milan)*, *53*, 1033-1038.

Goss, K. U. (2008), The pK(a) values of PFOA and other highly fluorinated carboxylic acids, *Environmental Science & Technology*, *42*(2), 456-458.

Hare, E. F., Shafrin, E. G., and Zisman, W. A. (1954), Properties of Films of Adsorbed Fluorinated Acids, *The Journal of Physical Chemistry*, *58*(3), 236-239.

Haszeldine, R. N. (1952), The reactions of metallic salts of acids with halogens. III. Some reactions of salts of fluorohaloacetates and of perfluoro acids, *J. Chem. Soc.*(Copyright (C) 2012 American Chemical Society (ACS). All Rights Reserved.), 4259-4268.

Hato, M., and Shinoda, K. (1970), Solubility and critical micelle concentrations of fluorinated surfactants in water, *Nippon Kagaku Zasshi*, *91*, 27-31.

Hilal, S. H., Karickhoff, S. W., and Carreira, L. A. (1995), A rigorous test for SPARC's chemical reactivity models: Estimation of more than 4300 ionization pK(a)s, *Quant. Struct.-Act. Relat.*, *14*(4), 348-355.

Kaiser, M. A., Larsen, B. S., Kao, C.-P. C., and Buck, R. C. (2005), Vapor Pressures of Perfluorooctanoic, -nonanoic, -decanoic, -undecanoic, and -dodecanoic Acids, *J. Chem. Eng. Data*, *50*, 1841-1843.

Katsushima, A., Hisamoto, I., Fukui, T., Kato, T., and Nagai, M. (1968), Polyfluoroalkyl acrylate polymers, edited, p. 5 pp., Daikin Kogyo Co., Ltd. .

Katsushima, A., Hisamoto, I., Nagai, M., Fukui, T., and Kato, T. (1976), Oil proofing and water proofing agents, edited, pp. 5 pp. Division of Japan. Koho 73 41,152., Daikin Kogyo Co., Ltd., Japan .

Kauck, E. A., and Diesslin, A. R. (1951), Some properties of perfluorocarboxylic acids, *J. Ind. Eng. Chem. (Washington, D. C.)*, *43*, 2332-2334.

Kawaguchi, S., Matsukawa, Y., Okamoto, S., Iwatani, S., and Murotani, E. (2009), The manufacturing method of fluorocarbons, and new fluorocarbons, edited, p. 15pp., Asahi Glass Co., Ltd., Japan .

Klamt, A. (2005), *COSMO-RS, From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design*, Elsevier.

Kometani, Y., Yoshimura, T., and Fujii, T. (1968), Colloidal polyfluoroolefins, edited, p. 3 pp., Daikin Kogyo Co., Ltd. .

Kutsuna, S., and Hori, H. (2008), Experimental determination of Henry's law constant of perfluorooctanoic acid (PFOA) at 298K by means of an inert-gas stripping method with a helical plate, *Atmos. Environ.*, *42*(Copyright (C) 2012 American Chemical Society (ACS). All Rights Reserved.), 8883-8892.

LaZerte, J. D., Hals, L. J., Reid, T. S., and Smith, G. H. (1953), Pyrolyses of the Salts of the Perfluoro Carboxylic Acids1, *Journal of the American Chemical Society*, *75*(18), 4525-4528.

Lines, D., and Sutcliffe, H. (1984), Preparation and properties of some salts of perfluorooctanoic acid, *J. Fluorine Chem.*, *25*, 505-512.

Manzara, A. P., Fan, W.-q., Stern, R. M., and Moore, G. G. I. (1998), Alpha-branched fluoroalkylcarbonyl fluorides and their derivatives, edited, p. 85 pp., Minnesota Mining and Manufacturing Co., USA .

Meissner, E., Myszkowski, J., Szymanowski, J., and Sobczynska, A. (1992), Synthesis and surface activity of sodium salts of branched perfluorocarboxylic acids and their analogs containing one chlorine atom, *J. Chem. Technol. Biotechnol.*, *55*, 273-276.

Meissner, E., Twardochleb, B., Milchert, E., Wroblewska, A., and Szymanowski, J. (2003), Estimation of foam forming properties and surface tension of fire-extinguishing agents, *Tenside, Surfactants, Deterg.*, *40*, 353-360.

Meissner, E., Pelech, R., and Milchert, E. (2006), Surface activity of sodium salts of perfluoroalkyl acids and their analogs with one chloride atom at the œâ position, *Inz. Apar. Chem.*, *45*, 90-91.

Nakayama, H. (1967), KRAFFT TEMPERATURES OF PERFLUORO-OCTANOIC ACID AND OF ITS SALTS, *Bull. Chem. Soc. Jpn.*, *40*(7), 1592-&.

Naonori, E., and Koji, T. (1985), Etchant composition, edited, p. 15 pp., Daikin Kogyo Co., Ltd., Japan .

Nishiyama, T. (1988), Preparation of n- and isoperfluorotetradecane mixture compositions as vapor-phase soldering solvents, edited, p. 6 pp., Shin Akita Kasei K. K., Japan .

Pennsalt Chemicals Corp (1963), Halogenated organic compounds, edited, p. 31 pp., Pennsalt Chemicals Corp.

Plashkin, V. S., Agishev, Y. N., Maksimova, V. P., Selitzev, Y. N., Krylov, A. I., Tataurov, G. P., Ryabinin, N. A., and Kazakov, V. Y. (1975), Perfluorinated carboxylic acids, edited, USSR .

Prokop, H. W., Zhou, H. J., Xu, S. Q., Wu, C. H., and Liu, C. C. (1989), Analysis of the products from the electrochemical fluorination of octanoyl chloride, *J. Fluorine Chem.*, *43*, 277-290.

Radell, J., Brodman, B. W., Hirshfeld, A., and Bergmann, E. D. (1965), - *69*(- 3), - 32.

Rayne, S., and Forest, K. (2010), Theoretical studies on the pKa values of perfluoroalkyl carboxylic acids, *J. Mol. Struct.: THEOCHEM*, *949*, 60-69.

Shinoda, K., Hato, M., and Hayashi, T. (1972), Physicochemical properties of aqueous solutions of fluorinated surfactants, *J. Phys. Chem.*, *76*, 909-914.

Stern, R. M., and Fan, W.-q. (1998), Aqueous film-forming foam compositions, edited, p. 81 pp., Minnesota Mining and Manufacturing Co., USA .

Syracuse_Research_Corporation (2000-2008), EPI Suite, edited.

Vanden, H. J. P., Thompson, J. T., Frame, S. R., and Gillies, P. J. (2006), Differential Activation of Nuclear Receptors by Perfluorinated Fatty Acid Analogs and Natural Fatty Acids: A Comparison of Human, Mouse, and Rat Peroxisome Proliferator-Activated Receptor-α, -β, and -γ, Liver X Receptor-β, and Retinoid X Receptor-α, *Toxicol. Sci.*, *92*, 476-489.

Von Werner, K., and Probst, A. (1987), Procedure for the preparation of perfluorocarboxylic acids and their use as tensides, soldering flux, and lubricants, edited, p. 7 pp., Hoechst A.-G., Fed. Rep. Ger. .

Wallington, T. J., et al. (2006), Formation of C7F15COOH (PFOA) and Other Perfluorocarboxylic Acids during the Atmospheric Oxidation of 8:2 Fluorotelomer Alcohol, *Environ. Sci. Technol.*, *40*, 924-930.

Washburn, S. T., Bingman, T. S., Braithwaite, S. K., Buck, R. C., Buxton, L. W., Clewell, H. J., Haroun, L. A., Kester, J. E., Rickard, R. W., and Shipp, A. M. (2005), Exposure Assessment and Risk Characterization for Perfluorooctanoate in Selected Consumer Articles, *Environ. Sci. Technol.*, *39*, 3904-3910.

Wroblewska, A., Meissner, E., and Milchert, E. (2006), Synthesis of technically useful perfluorocarboxylic acids, *J. Fluorine Chem.*, *127*, 345-350.

Yamada, T., and Higaki, J. (1993), Synthetic lubricants containing branched perfluoroalkyl esters for magnetic recording media, edited, p. 6 pp., Nisshin Fine Chemical Kk, Japan .

ANNEX

Table A.1. List of PFOA Precursors (from Environment Canada).

Name	CAS RN	Molecular formula	Listing (DSL or NDSL)
2-Propenoic acid, 2-methyl-, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl ester, polymer with 2-propenoic acid	53515-73-4	$(C_{15}H_{11}F_{15}O_4)_x$	DSL
Propanamide, 3-[(γ-ω-perfluoro-C_{4-10}-alkyl)thio] derivatives	68187-42-8	NA	DSL
Poly(difluoromethylene), a-fluoro-ω-[2- [[2-(trimethylammonio)ethyl]thio]ethyl]-, methyl sulfate	65530-57-6	NA	DSL
Poly(difluoromethylene), a,a'-[phosphinicobis(oxy-2,1-ethanediyl)]bis[ω-fluoro-	65530-62-3	NA	DSL
Poly(difluoromethylene), a-fluoro-ω-[2-(phosphonooxy)ethyl]-	65530-61-2	NA	DSL
Thiols, C_{8-20}, γ-ω-perfluoro, telomers with acrylamide	70969-47-0	NA	DSL
Carbamic acid, [2-(sulfothio)ethyl]-, C-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) ester, monosodium salt	82199-07-3	NA	DSL
Carbamic acid, [2-(sulphothio)ethyl]-, C-(γ-ω-perfluoro-C_{6-9}-alkyl) esters, monosodium salts	95370-51-7	NA	DSL
1,3-Propanediol, 2,2-bis[[(γ-ω-perfluoro-C_{4-10}-alkyl)thio]methyl] derivatives, phosphates, ammonium salts	148240-85-1	NA	NDSL
1,3-Propanediol, 2,2-bis[[(γ-ω-perfluoro-C_{6-12}-alkyl)thio]methyl] derivatives, phosphates, ammonium salts	148240-87-3	NA	NDSL
Thiols, C_{4-20}, γ-ω-perfluoro, co-telomers with acrylic acid and acrylamide	NA	NA	Not listed
1-Decanol, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro (or 1,1,2,2-tetrahydroperfluoro-1-decanol or 8:2 fluorotelomer alcohol)	678-39-7	$C_{10}F_{17}H_5O$	DSL
Octanoyl fluoride, pentadecafluoro-	335-66-0	$C_8F_{16}O$	NDSL
Octanoic acid, pentadecafluoro-, methyl ester	376-27-2	$C_9H_3F_{15}O_2$	NDSL
Octanoic acid, pentadecafluoro-, ethyl ester	3108-24-5	$C_{10}H_5F_{15}O_2$	NDSL
8:2 Fluorotelomer acrylate polymers[2]	NA	NA	NA
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-iododecane (C8-2 iodide)	2043-53-0	NA	NA
2-propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl methacrylate (C8-2 methacrylate)	1996-88-9	NA	DSL
2-propenoic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl acrylate (C8-2 acrylate)	27905-45-9	NA	DSL
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodec-1-ene (C8-2 olefin)	21652-58-4	NA	NA
Phosphoric acid surfactants (e.g., 8:2 polyfluoroalkyl phosphoric acid diester or 8:2 diPAP)[4]	NA	*x*:2 diPAP $(F(CF_2)_xCH_2CH_2O)_2P(O)OH$	NA
Perfluorooctylsulfonamides[3]	NA	$F[CF_2]_8SO_2NRR'$ where R and R' can be CH_2CH_2OH, CH_3, CH_2CH_3, or H	NA
1,3-Propanediol, 2,2-bis[[(γ-ω-perfluoro-C10-20-alkyl)thio]methyl] derivs., phosphates, ammonium salts	148240-89-5	NA	NDSL
Oxirane, methyl-, polymer with oxirane, mono[2-hydroxy-3-[(γ-ω-perfluoro-C8-20-alkyl)thio]propyl] ethers	183146-60-3	NA	NDSL
Poly(difluoromethylene), a-fluoro-ω-(2-sulfoethyl)-	80010-37-3	NA	NDSL
2-Propenoic acid, 3,3,4,4,5,5,6, 6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl ester, polymer with 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl 2-propenoate, alpha-(2-methyl-1-1-oxo-2-2-propenyl)-omega-[(2-methyl-1-oxo-2-propenyl)oxy]poly(oxy-1, 2-ethanediyl), 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10, 11,11,12,12,13,13,14,14,15,15,16,16,16-nonacosafluorohexadecyl 2-propenoate, octadecyl 2-propenoate, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,	116984-14-6	NA	not listed

10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl 2-propenoate and 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,18,18-tritriacontafluorooctadecyl 2-propenoate			
Pentanoic acid, 4,4-bis[(γ-ω-perfluoro-C8-20-alkyl)thio]derivs., compds. with diethanolamine	71608-61-2	NA	NDSL

KLIMA- OG FORURENSNINGS- DIREKTORATET

Klima- og forurensningsdirektoratet
Postboks 8100 Dep, 0032 Oslo
Besøksadresse: Strømsveien 96
Telefon: 22 57 34 00
Telefaks: 22 67 67 06
E-post: postmottak@klif.no
Internett: www.klif.no

Utførende institusjon	ISBN-nummer
Senter for teoretisk og beregningsbasert kjemi (CTCC), Kjemisk institutt, Universitetet i Oslo	

Oppdragstakers prosjektansvarlig	Kontaktperson i Klima- og forurensningsdirektoratet	TA-nummer
Claus Jørgen Nielsen	Marit Kopangen	2944/2012
		SPFO-nummer

	År	Sidetall	Klima- og forurensningsdirektoratets kontraktnummer
	2012	58	3012013

Utgiver	Prosjektet er finansiert av
Klima- og forurensningsdirektoratet	Klima- og forurensningsdirektoratet

Forfatter(e)
Claus Jørgen Nielsen

Tittel - norsk og engelsk

PFOA isomerer, salter og forløpere. Litteraturstudie og vurdering av fysisk-kjemiske egenskaper

PFOA Isomers, Salts and Precursors, Literature study and evaluation of physico-chemical properties

Sammendrag – summary

Rapporten gjennomgår litteraturen om fysisk-kjemiske egenskaper ved PFOA, inkludert strukturelle isomerer og deres ammonium-, natrium-, kalium- og sølvsalter, som er referert i CAS nummer register databasen.

The literature on PFOA including its structural isomers and their ammonium, sodium, potassium and silver salts referenced in CAS# registry database has been reviewed with respect to physico-chemical properties.

4 emneord	4 subject words
PFOA, fysisk-kjemiske egenskaper	PFOA, Physico-chemical properties